Low Cost Microengineered Functional IR Material

Final Report

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REPORT TITLE: Low Cost Microengineered Functional IR Material

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Sincerely,

A.M.

Dr. Albert M. Green
Deputy Director, Technology
Development Laboratories

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SECTION 1: GENERAL INFORMATION

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
12/1/00

3. REPORT TYPE AND DATES COVERED
Final Report – 9/26/97 – 10/31/99

4. TITLE AND SUBTITLE
Low Cost Microengineered Functional IR Material

5. FUNDING NUMBERS
C DAAG55-97-C-0055

6. AUTHORS
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Science Applications International Corporation
1710 SAIC Drive, MS 2-3-1
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
ARO 37665.1-PH

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

DISTRIBUTION STATEMENT A
Approved for Public Release
Distribution Unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

This report documents an approach to fabricating large area, low cost 3-D photonic crystal structures using continuously web compatible techniques. We document and detail a process that involves microembossing, differential stripping, direct transfer, and alignment. We also discuss an analytical technique that can be used to model the reflectance and trasmittance of multilayer structures.

14. SUBJECT TERMS
embossing, lamination, photonic crystal, liftoff, alignment, continuous web

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

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1.0 Summary

The principle goal of SAIC's Highly Controlled Dielectric Emissivity (HIDE) program was to apply the techniques of large area, low cost, continuous web manufacturing to fabricate photonic band gap structures that exhibit finite width pass- and stop-band properties in the 8-12 μm wavelength regime. The 3 major thrusts of the program were:

(1) Develop web compatible techniques for manufacturing single layer periodic structures
(2) Develop techniques that can be used to stack, or layer, the single layer structures
(3) Develop a theoretical framework for understanding the performance of the fabricated structures

We developed several innovative techniques to fabricate single layer structures. All of these approaches centered on the use of microembossed structures which can be fabricated over very large areas at low cost. The most important technique, direct transfer, can be used to fabricate 3 dimensional structures (we used hemispheres) in one substrate and transfer them to another surface.

We also developed techniques for layering structures. We were able to fabricate structures of up to 10 layers. We concluded that rotational alignment is possible, however, we were not able to successfully achieve translational alignment.

Finally, we developed a semi-analytic integral equation approach for the computation of the reflection and transmission coefficients of a periodic single or multilayer array of dielectric or metallic spheres inside a host medium, which may be lossy.

The program was divided into 3 phases. Phase 1 (10/97 – 5/98) has been completed and focused on developing the appropriate microembossing, and liftoff procedures to fabricate a single layer with the proper periodicity. Phase 2 (5/98 – 5/99) focused on developing tools and techniques multilayer fabrication. In Phase 3 (6/98 – 10/99), we continued development on multilayer techniques to produce multilayer photonic crystal structures. The report below summarizes our fabrication and modeling efforts.

The participating scientific personnel is listed below:

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2.0 Fabrication

Our basic approach involves single layer fabrication of periodic dielectric structures that can be layered to form a photonic crystal. The ultimate goal is to produce materials using our continuous web techniques that exhibit a photonic bandgap in the 8-12 μm (1250 – 800 cm^{-1}) regime.

Preliminary work revealed a somewhat difficult materials issue, namely most of the conventional materials used in embossing technology such as polycarbonate and CAB(cellulose acetate butyrate) have significant absorbing properties in the 8 - 12 μm region. After an extensive literature and database search, we identified two materials as suitable matrix materials for the final structures, polyethylene and a material known as Poly IR2 which is a proprietary polymeric product of Fresnel Technologies, Inc and is used to fabricate Fresnel Lenses for 8 - 12 μm. These materials are thermally embossable and moldable. Unlike polycarbonate and CAB, solvent embossing with conventional solvents at room temperature did not seem possible because of solubility limits. It should be pointed out that the availability of soluble polymer is not essential for achieving the ultimate goals of the program. For purposes of developing evaluation prototypes, however, the ability to use cast films that are spun or rod coated would provide an extra degree of freedom and considerably more flexibility in the planarization step.

Early in the program we evaluated the materials issue more carefully as part of developing the fabrication process. The principal purpose of this evaluation was to determine the range of polymeric materials that do not have significant absorbance in the wavelength region of interest and, based on previous experience, can be fabricated in a web compatible process. These considerations drove many of the fabrication approach decisions throughout the program and are worth a separate discussion below.

2.1 Substrate Infrared Spectra

For HIDE fabrication, a principle considerations were infrared spectra vis a vis the absorption in 8-12 μm and the solubility. The results are summarized below.

There are a number of commercially available libraries either in printed or electronic form that provides infrared absorption characteristics of materials. The purpose of these databases is primarily for compound identification via the various absorption peaks. As such, the listed spectra are normalized to absorption peak height and not material thickness so do not provide an absolute measure of optical absorbance. Nonetheless, since we were interested in materials which have *no peaks* in the 8 - 12 μm range, we believed the database is a useful guide.

Unfortunately, the cost of ownership of such a database was much higher than is justified by this investigation. It was possible; however, to convince Nicolet Instruments who are purveyors of the electronic form of these databases to conduct a one time, no-charge search of the databases most germane to our goals. The search criterion was simply no absorption peaks in 8 - 12 μm region. Three databases were searched representing about 15,000 organic compounds. A complete listing of the compounds searched will be submitted in the final report. 12 compounds were listed as the best fit to the search criteria. The following compounds were considered the best candidates for web compatible fabrication consistent with the HIDE goals.

Poly(ethylene) $\eta = 450$ cps(viscosity)
Poly(ethylene) $\eta = 6000$ cps
Poly(1-hexadecene) isotatic
Poly(ethylene:propylene:diene) 70% ethylene, 4% diene
Poly(styrene:butadiene)ABA block (28% styrene)
Poly(ethylene:acrylic acid) 10% acrylic acid
Poly(ethylene:propylene:diene) 70% ethylene, 4% diene(repeated)
Poly(ethylene:acrylic acid) 10% acrylic acid(repeated)
Paraffin wax #1
Poly(1-butene) isotactic, high MW
Versamine 551
Thixtrol SR-100

Of these compounds, the last two, versamine and thixatrol are polymer additives. Versamine is a product of the Henkel Corporation and is a curing agent for epoxy coatings. Thixtrol is a product of Rheox, Inc and is a thixatropic additive to control viscosity of liquid materials like paint.

With the exception of the styrene:butadiene copolymer, the remainder all fall into the general family called polyolefins which include polyethylene and polypropylene. The distinguishing feature of these compounds with regard to their IR spectra is that regardless of whether the polymer is linear or branched, the entire molecule contains only two chemical bonds, C-C or C-H. The result is absorption bands at 3.5, 7, and 14μ.

Paraffin which is a short chain polyolefin with a chain length of about 15-40 carbons shows the typical IR absorption spectra for this kind of material. An excellent introduction to the properties of polyolefins can be found at **http://www.umr.edu/~wlf/CHEM381/chap22.html**

We measured the transmission of a number of substrates to determine their suitability for use in the program. Figure 2.1.1 shows the transmission spectra of 2.0 mils of polyethylene.

2.2 Substrate Solubility

We focused on Polyethylene due to its low absorption in 8-12μm. Polyethylene is relatively insoluble in most solvents, in fact it is sometimes used to make gasoline containers. The literature claims that it has some solubility in hot o-xylene and CS_2. We performed experiments that showed very little indication of solubility with a variety of solvents at room temperature. A possible alternative is paraffin. We have obtained the highest melting grade from Aldrich. This material is a hard, brittle material with a milky appearance. We were able to produce saturated solutions by dissolving this material in petroleum distillates such as petroleum ether at 60°C. At this point we believe that normal polyethylene can be softened with the same solvents at elevated temperatures.

From this analysis, we concluded that in general, there is a very limited selection of materials that can be used for the lattice element in these structures and in particular organic materials. Simple polyethylene film has the correct absorbing properties but suffers from limiting mechanical properties. There are basically two kinds of polyethylene high-density polyethylene (HDPE) and the low-density variant (LDPE). The difference is the result of the degree of polymer branching cf. Appendix I. LDPE is relatively soft. We found that it was very difficult to main reasonable dimensional integrity following the embossing process. Low density is more rigid but also said to suffer from shrinkage associated with molding although we have not tried to emboss this material.

Although we do not know the exact composition of Poly IR2 it is reasonable to assume it is also a variant of polyethylene. We obtained Poly IR2 samples and found them to be waxy and milky appearance. We presumed that is probably a polyethylene copolymer where the amount of additive has been adjusted to balance improvements in mechanical properties and UV stability against loss of in band transmission.

Given the nature of the final structure which is expected to begin with a fairly rigid base sheet on which is the lattice is fabricated, we expect that base will be either HDPE or Poly IR2. Filling or leveling the lattice with either low melting PE or paraffin have been our materials of choice.

2.3 Fabrication Procedure

The basic substrate fabrication procedure for multiple layers involves the following steps.

(1) Fabrication of master and embossing tool
(2) Microembossing
(3) Release layer deposition
(4) Metal deposition and differential stripping
(5) Interlayer deposition and transfer (and align) of structures from donor substrate (polycarbonate) to substrate of choice (polyethylene)

We highlight the important steps in the discussions below. The microembossing procedure is a previously developed Polaroid/MicroContinuum trade secret.

2.3.1 Master Fabrication

The procedure used for fabricating the embossing tool master is as follows:
(1) Coat photoresist on glass
(2) Expose with 3-beam interference pattern with the pitch determined by beam angles
(3) Modulate exposure and develop to control degree of hole opening and depth
(4) Create embossing photoresist master

Figure 2.3.1.1A and 2.3.1.1B are SEMs of a master fabricated in the above fashion.

2.3.2 Microembossing

Microembossing is a technology for "stamping" lithographically defined features into a substrate of choice. The advantage is that it offers very high resolution and is highly reproducible. In addition, we have argued that it is one of the few choices for large area, low cost fabrication of single layer, a potentially multiple layer 3-D photonic crystal structures. While not applicable to this program, it should be pointed out that the embossing/liftoff procedures we demonstrate for micron scale features has also been demonstrated for100 nm size features.

We successfully embossed polyethylene using a thermal process, and CAP and polycarbonate using a chemical process. Both of these processes were developed using processes that are proprietary to Polaroid and MicroContinuum.

2.3.3 Release Layer

The central purpose of the release layer is to allow for regions of the metallic overlayer to be precisely and repeatably separated from the underlying substrate leaving behind a 3-D periodic structure. We performed an exhaustive literature search and many trial and error attempts to determine the proper release agent. The best results were obtained using a dilute, aqueous solution of cationic detergent that coats the surface with a very thin (sub micron) residue allowing separation of the metal. Our liftoff experiments were performed with Indium. Indium was originally chosen because it has a low vaporization temperature and seemed to be most suitable for differential stripping evaluation studies. We believe the use of detergent-based release agents can be used to differentially strip most metals using the techniques described.

2.3.4 Differential Stripping

Differential stripping is performed by pressing the donor substrate and adhesive layer between 2 rollers and then pulling them apart. We tried a number of different rolling pressures and adhesives to determine the proper combinations. We found that regular scotch tape was the best adhesive. This appeared to be almost pressure insensitive. Figure 2.3.4.1 illustrates the differential stripping process, and the importance of geometry to produce the required effect. In particular, the process works because the adhesive does not come into contact with the metal in the cups, and hence is left behind when the adhesive is removed. Figure 2.3.4.2A shows a surface that has been differentially stripped. Figure 2.3.4.2B shows the complimentary liftoff layer. It should be pointed out that this process was extremely reproducible and we were able to demonstrate excellent differential stripping over virtually the entire sample area (~4 in^2).

The importance of geometry in the differential stripping process cannot be over emphasized. We had a series of failures in the stripping process that were eventually tied to a faulty master. Figures 2.3.4.3A and 2.3.4.3B is an SEM of the master used to fabricate structures that did not adequately strip. The embossing master shows the features that will be embossed in a substrate using the corresponding embossing tool. Although we experienced a major delay associated with this failure, it caused us to carefully examine the stripping process. We concluded that the process works only for "sharply" defined aspect ratios. Differential stripping works for the hemispherical geometries we explored because less material is deposited along the ring of the hemisphere allowing it to fracture in the region of interest, and thus differentially strip as needed.

2.3.5 Layer Stacking

Two issues dominate the procedures that can be considered for stacking of individual layers to form a 3-D structure. First, the substrate thickness on the layers to be stacked, such as those shown in figure 2.3.4.2A are ~1 mil (25 μm), which is much thicker than a lattice constant. And second, polyethylene substrates of interest do not have good dimensional stability. This severely limits the ability to effectively align the substrates.

Considering these limitations, we developed a technique for stacking structures that we refer to as "direct transfer". The procedure is as follows:

(1) Begin with the single layer structures as shown in figure 2.3.4.2A
(2) Fill cups with acqueos dispersion of polyethylene polymer coating using wire-wound coating rod. The filling is controlled by the solution concentration and wire guage of the coating rod.
(3) Transfer to receiving sheet.

Figure 2.3.5.1 illustrates the procedure.

Figure 2.3.5.2 are structures that has been transferred to a receiving sheet using the procedure described. Figure 2.3.5.3 is a cross sectional view the substrate that has been

planarized as described in step (2) above. Figure 2.3.5.4A and 2.3.5.4B show the size over which structures can be transferred. Each of the features represents a "cup" that has been transferred from the donor to the receiver sheet.

We had a great deal of success using this procedure. In particular, we found it was relatively easy to control the interlayer thickness as well as to reproducibly transfer large areas from the donor sheet to the receiving sheet.

The procedure has important advantages compared to other approaches we considered. Most importantly, since the microembossed structure is not incorporated into final photonic crystal structure, it can be optimized for it's microembossing, mechanical, and temperature properties. We believe that the transfer procedure is the most important contribution to the HIDE program by the SAIC team.

We built up 3-D photonic crystal structures using this procedure. Figure 2.3.5.5 shows a multilayer stack that has been built up by combining the steps discussed above. To obtain this image, we cut a multilayer structure with a razor blade and looked for regions that had been cut and lifted up. Multiple regions can be seen along the cut line. For example, figure 2.3.5.6 shows a region where the top layer has separated and curled back from the layers below. The features that look surprisingly like octopus tentacles are the underside of the upper layer. Figure 2.3.5.7 is a high magnification image of a single layer. Notice how thin the interlayer spacing can be made.

Figure 2.3.5.8 shows a potential difficulty with the fabrication procedure described. We were concerned that the stacking process would crush the structures below the top layer. Figure 2.3.5.8 was created by applying the same pressure and heat treatment (both of which are low) used in building up the structure layer by layer. The hemispherical structures are flattened somewhat. We explored the possibility of changing the filling material, however this was not possible in view of the time and budgetary constraints.

2.3.6 Alignment

Alignment of the layers is the greatest challenge to the fabrication procedure described. The initial goal was to create zincblende lattice structures by stacking individual layers arranged in a hexagonal array. This approach requires 6 layers to complete a unit cell with the zincblende structure "grown" in the [111] direction. Figure 2.3.6.1 describes and illustrates the stacking procedure.

We explored several approaches to layer alignment. The primary difficulty is the fact that the layer and substrate must be exceptionally rigid to allow for submicron alignment over wafer size substrates. We settled on a procedure that involved transfer of structures to a rigid glass substrate and aligning subsequent layers to software generated "fiducials". There steps were:

(1) Fuse bottom layer to glass base.

(2) Align next layer by racking focus between top and bottom layers and using software ficucials and features (defects) at the edge of the pattern. This specific step is possible because of the many reproducible features at the edge of the pattern. These features are the same for all layers fabricated from the same master.
(3) Fuse layers and repeat.
(4) Transfer structure off of rigid glass substrate using predeposited release layer.

Figures 2.3.6.2A and 2.3.6.2B show several fiducials that are marked and aligned by a software image processing program.

Maintaining the layer dimensions (i.e., not stretching) while properly holding the sample so that it can be maneuvered into position are mutually exclusive and we developed several generation of alignment tools. Figure 2.3.6.3 shows the final setup used. This configuration allowed us to examine the diffraction pattern of a He-Ne laser impinging on the surface, as well as obtain high magnification images of surface features. As mentioned above, these features, which are reproduced on each layer, were used as fiducials for layer alignment. Figure 2.3.6.4 is a rendered drawing of the alignment tool. The tool allowed for both translational and rotational alignment.

We performed numerous alignment experiments using a variety of techniques. Our conclusion is that while rotational alignment is possible, translational alignment is extremely difficult.

3.0 Test and Measurement

We measured both single layer and multilayer structures. The single layer structures showed general agreement between predictions and measurements. Figure 3.0.1 shows the results for the polyethylene substrate and interlayer (recall the interlayer is a polyethylene aqueous solution) and for the single layer hex structures (such as those shown in section 2.3.5). The high angle disagreement between experiment and theory is likely due to surface roughness and the fact that the sample is partially blocked by the sample holder at high angles.

These measurements were performed using a CO_2 laser and selecting different wavelengths within the available 9-11μm band. A sketch of the setup is shown in figure 3.0.2.

We also performed measurements of the multlayer structures (in collaboration with SRI). These results were inconclusive.

4.0 Modeling and Simulation

The theoretical effort focused on formulating a semi-analytic integral equation for the computation of the reflection and transmission coefficients of a periodic single or multilayer array of dielectric or metallic spheres inside a host medium, which may be lossy. The results of this effort show that this method is equivalent to that of applying the

boundary conditions at the surface of the spheres, but it has the advantage that it provides an easy transition from the real to the spectral domain, where the convergence of the computed quantities is much faster. In a three dimensional lattice, we developed two for computing the dispersion relation of the photonic crystal. The reflection and transmission coefficients can be computed for a single or multilayer array of spheres embedded in a slab. Due to the small size of the matrices involved in the computations and the fast convergence, there is a small requirement for computer memory and time. The attached article, which has not been submitted for publication summarizes the theoretical results.

Figure 2.1.1

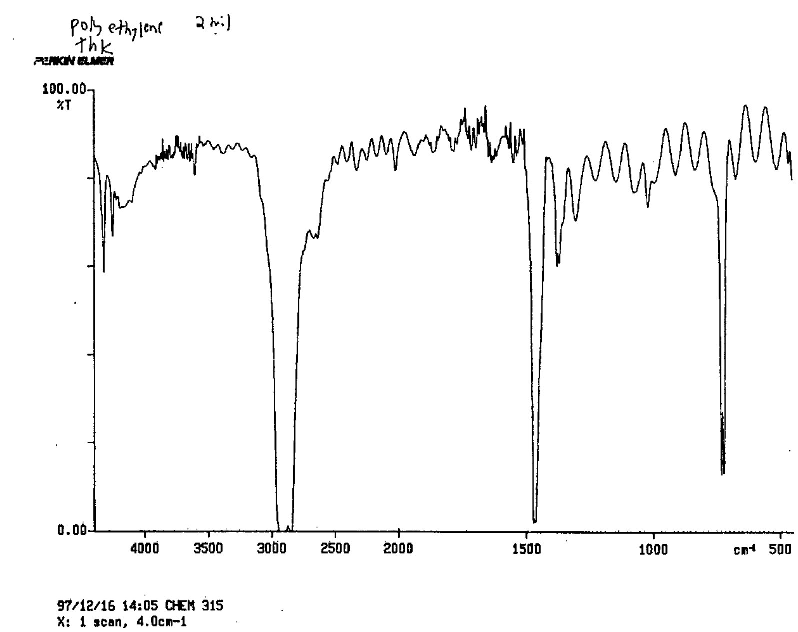
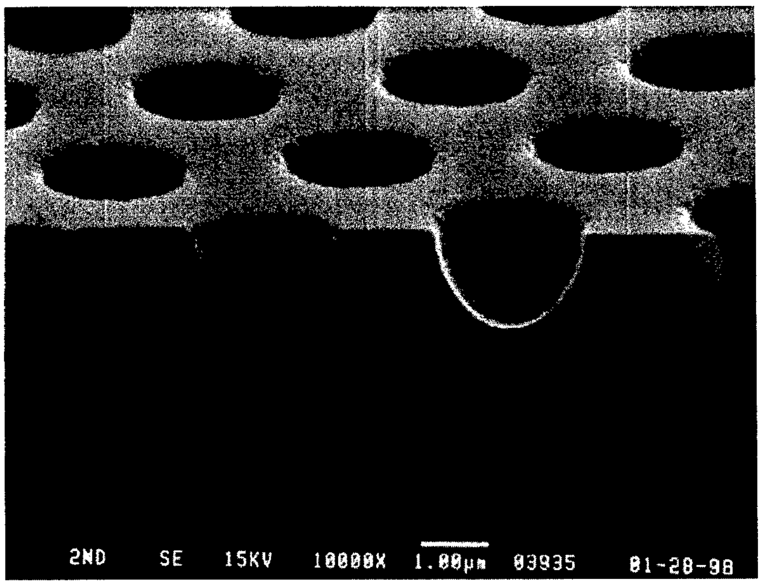


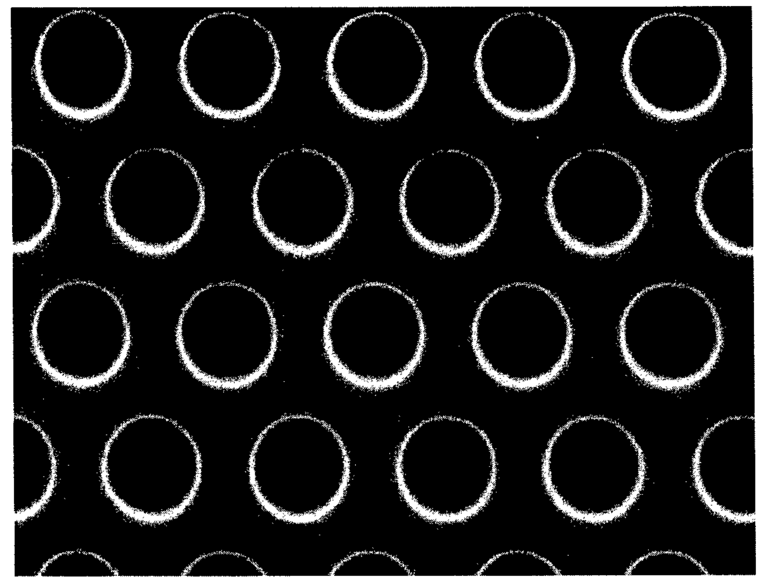
Figure 2.1.1: Polyethylene transmission spectra

Figures 2.3.1.1

A



B



Figures 2.3.1.1A and B: Microembossing masters

Figure 2.3.4.1

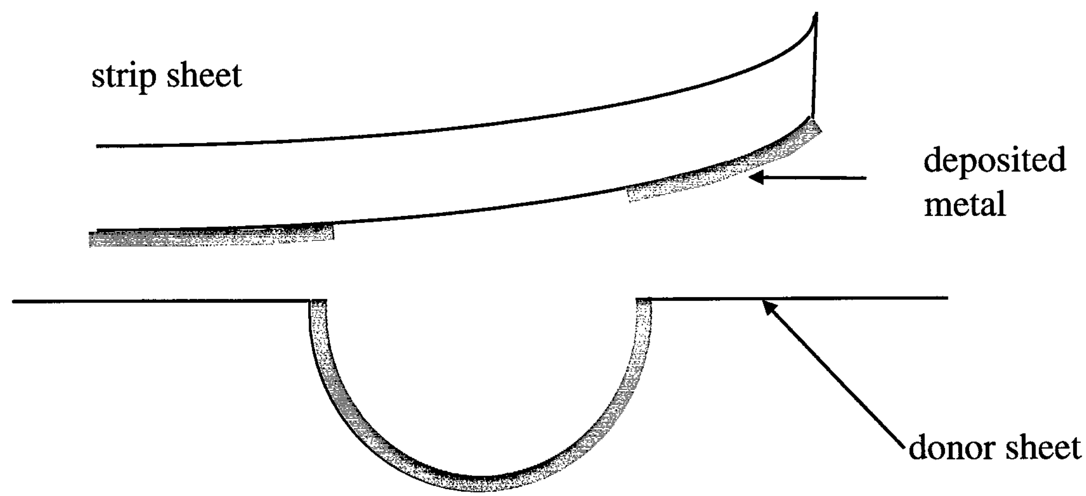
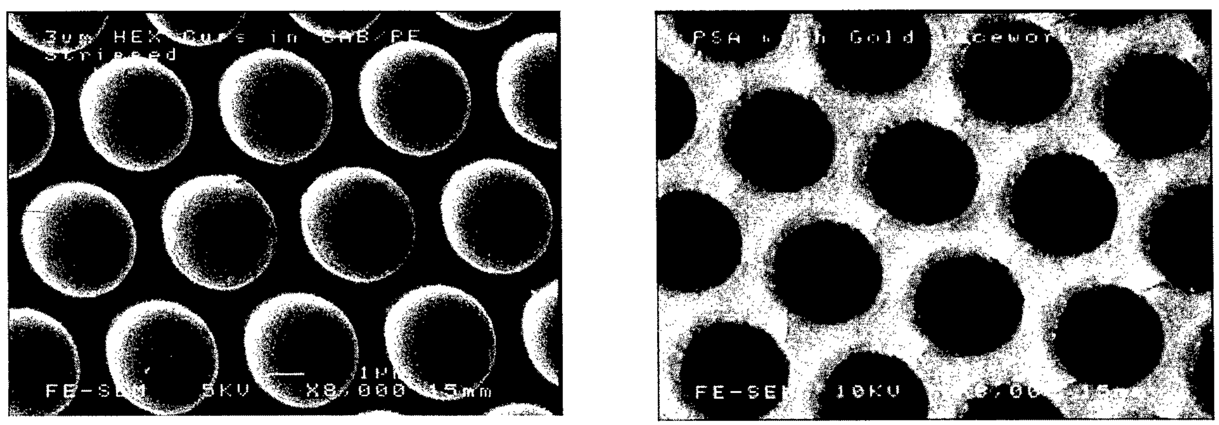


Figure 2.3.4.1: The differential stripping process

Figures 2.3.4.2

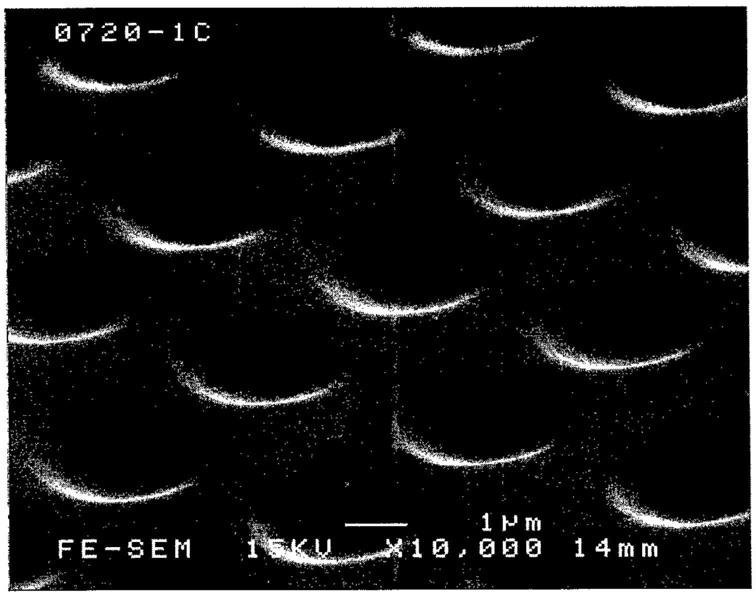
A B



Figures 2.3.4.2: A surface that has been differentially stripped (A) and the complimentary liftoff layer (B)

Figures 2.3.4.3

A



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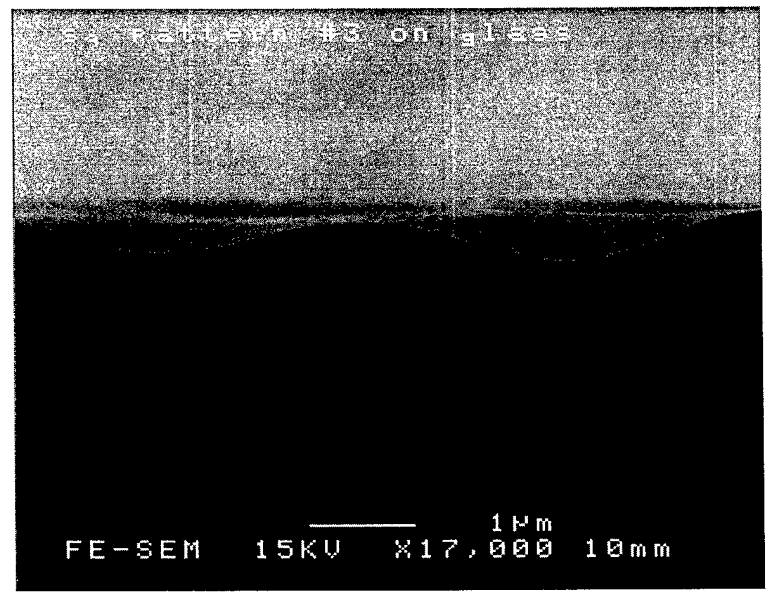
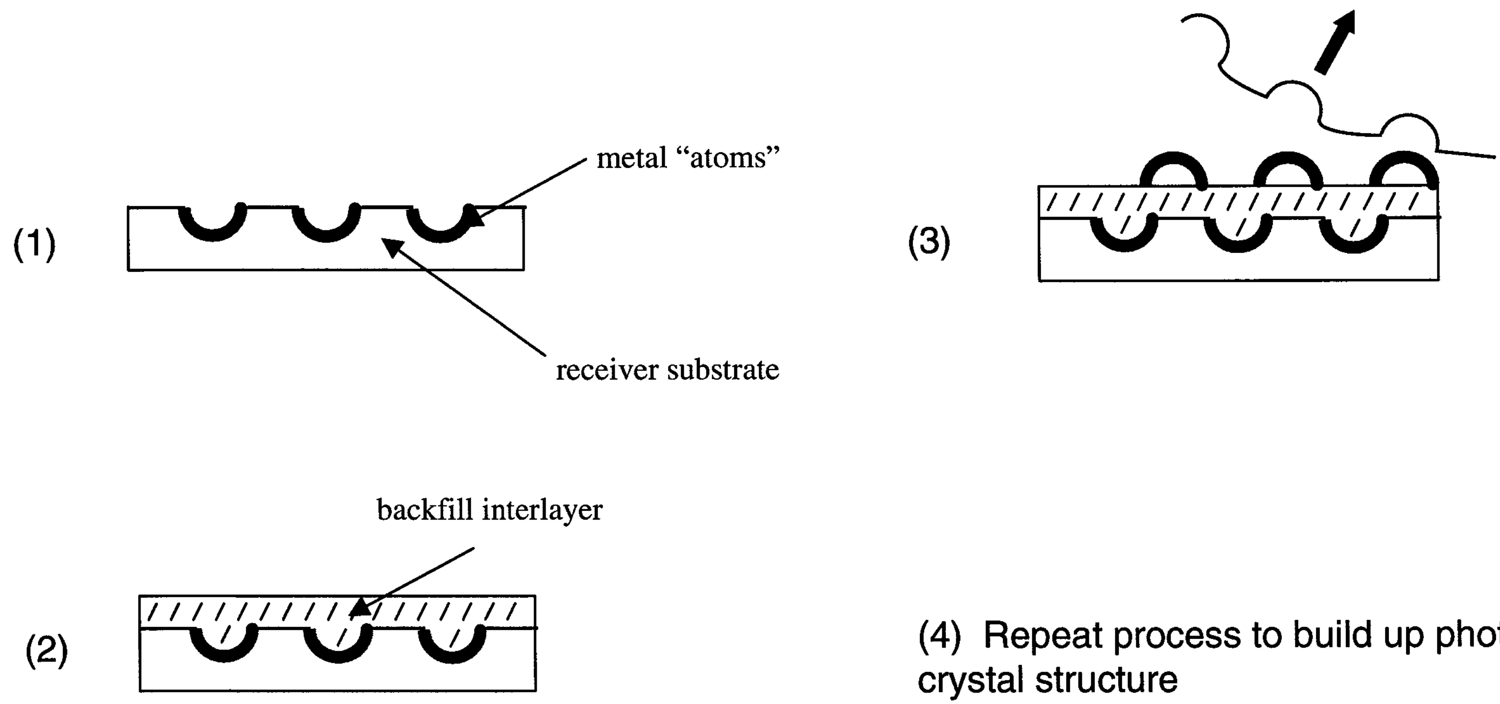


Figures 2.3.4.A and B: Embossing masters used to emboss substrates that did not differentially strip.

Figures 2.3.5.1



(4) Repeat process to build up photonic crystal structure

Figures 2.3.5.1: Procedure for fabricating multilayer structures

Figure 2.3.5.2

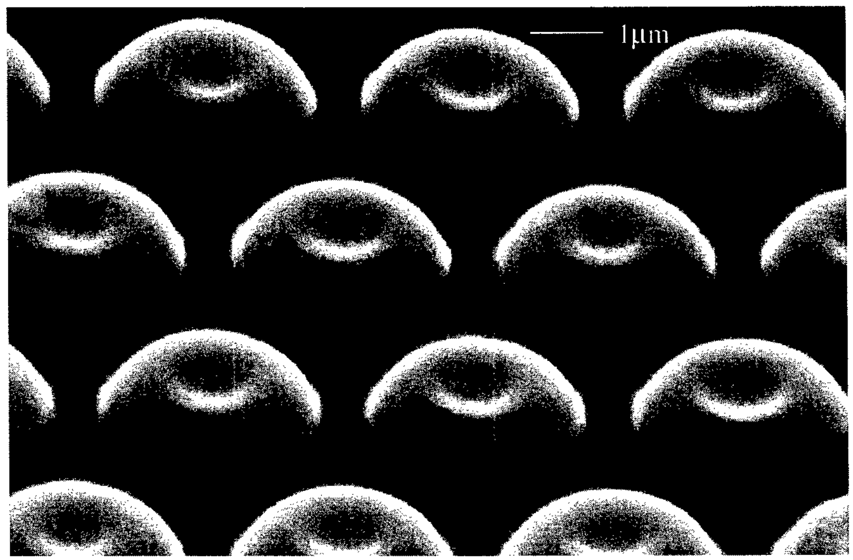


Figure 2.3.5.2: Structures that have been transferred from a donor sheet to a receiving sheet using the direct transfer process

Figure 2.3.5.3

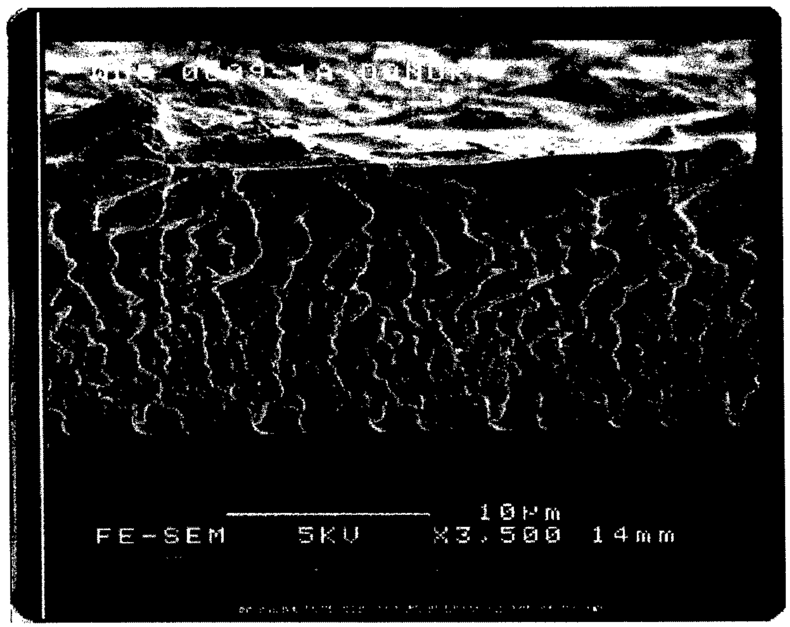
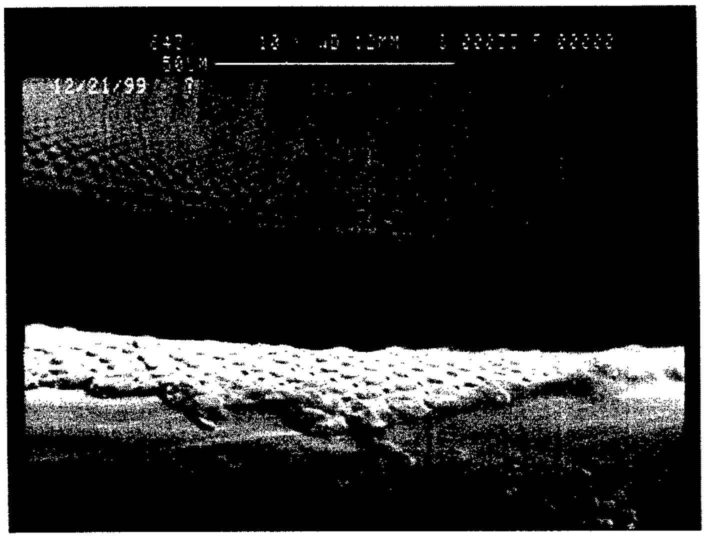


Figure 2.3.5.3: The interlayer used in the direct transfer process

Figures 2.3.5.4

A



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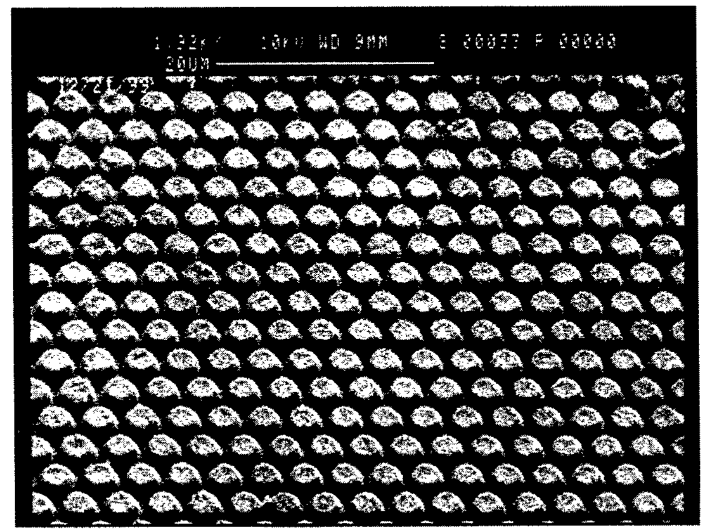


Figures 2.3.5.4A and B: Large area direct transfer with interlayer

Figure 2.3.5.5

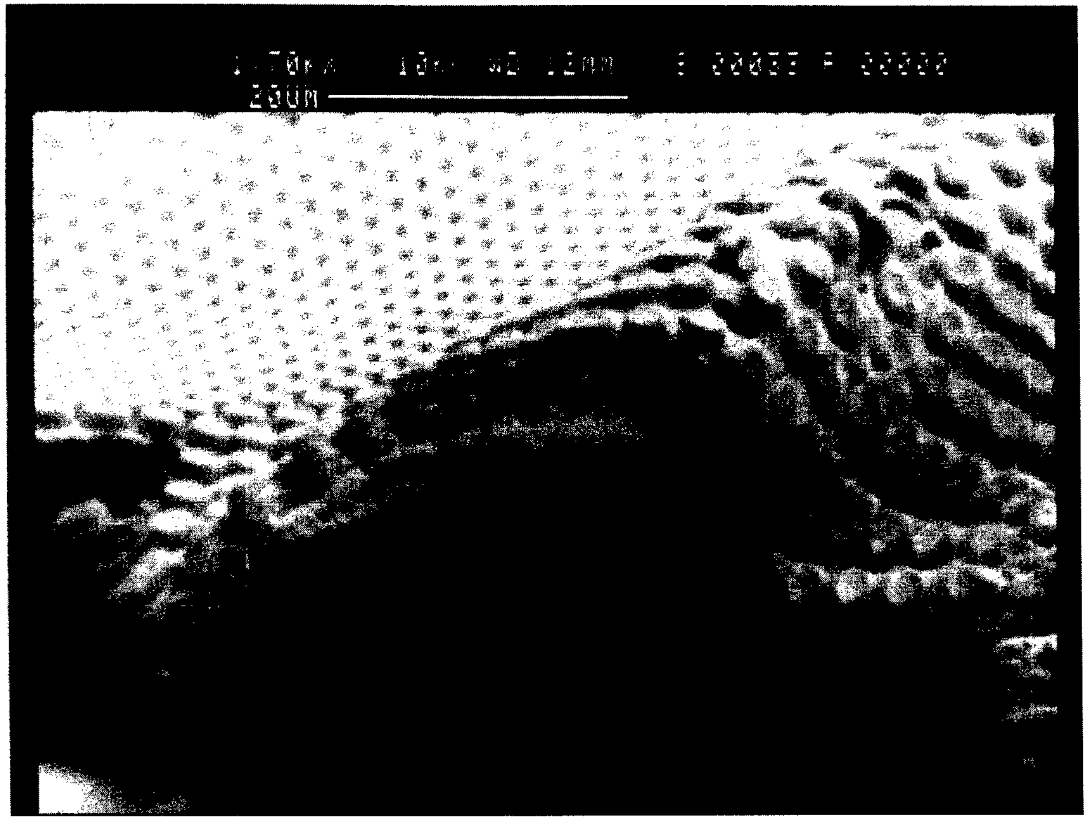


Figure 2.3.5.5: Multilayer structure

Figure 2.3.5.6

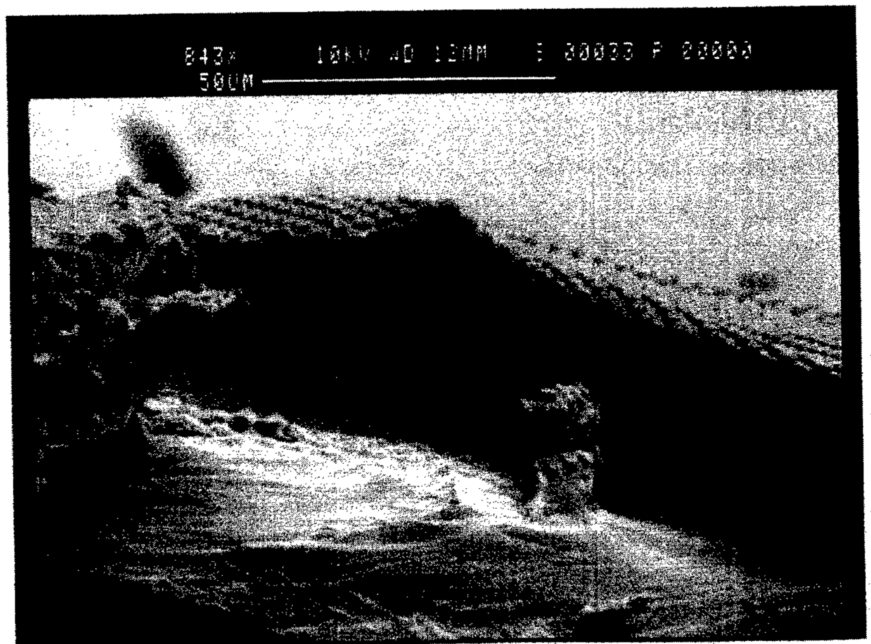


Figure 2.3.5.6: Lifted off top layer shows how thin the interlayer spacing can be made

Figure 2.3.5.7

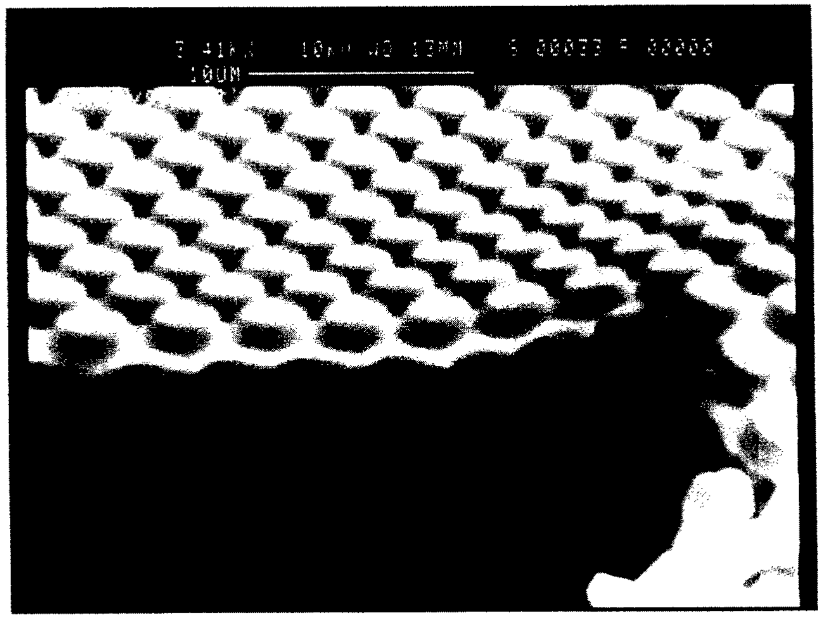


Figure 2.3.5.7: High magnification of the top layer illustrates how thin the interlayer can be made

Figure 2.3.5.8

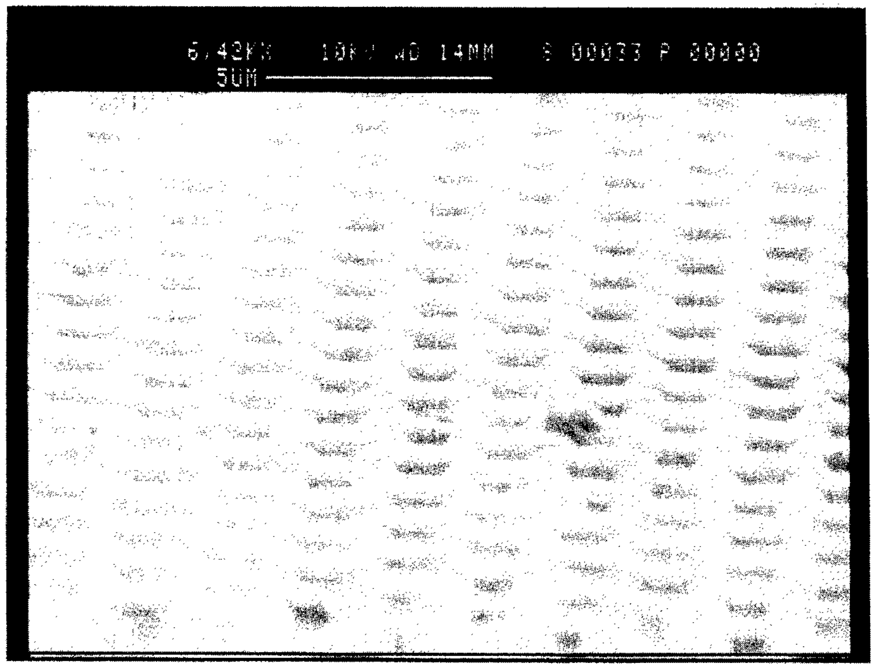
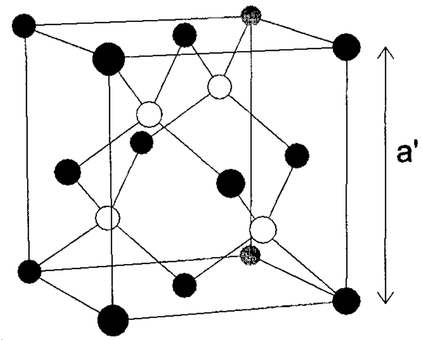


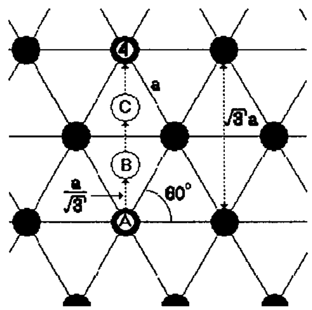
Figure 2.3.5.8: The stacking process can potentially crush the features in lower layers

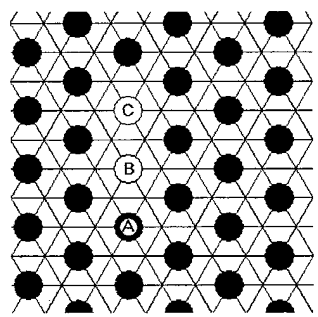
Figures 2.3.6.1

"Atom" spacing versus cell height:

$$a = \frac{a'}{\sqrt{2}}$$







Separation between layers:

X′ ⟶ Y:

$$\Delta v' = \frac{a}{2\sqrt{6}} = \frac{a'}{4\sqrt{3}}$$

X ⟶ X′:

$$\Delta v = \frac{\sqrt{3}}{4} a' = \sqrt{\frac{3}{2}}\frac{a}{2}$$

- Individual layers consist of "atoms" arranged in a hexagonal array
- a is separation between "atoms" in the sheet; a' is height of unit cell
- Stacking in [111] direction for hexagonal sheets
- 6 layers required for a unit cell
- Layers stacked in AA′BB′CC′ pattern:
  – Layer A′ directly over layer A
  – Layer B shifted so "atoms" centered in triangle of AA′ layers
  – Layer B′ directly over layer B
  – Layer C shifted so "atoms" centered in triangle of BB′ layers
  – Layer C′ directly over layer C

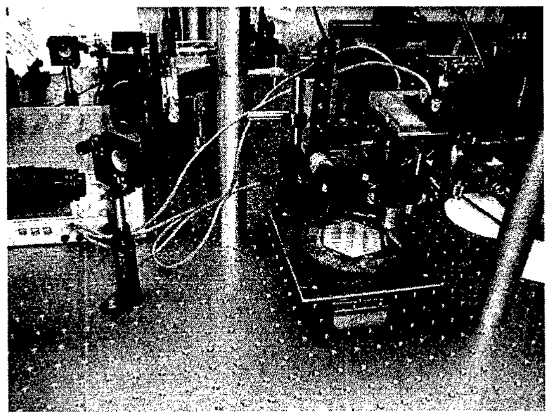
Figures 2.3.6.2

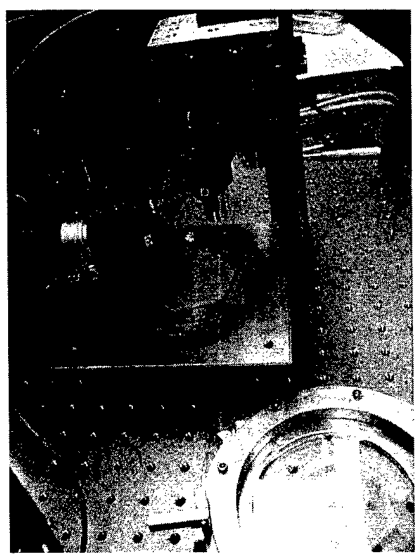
A

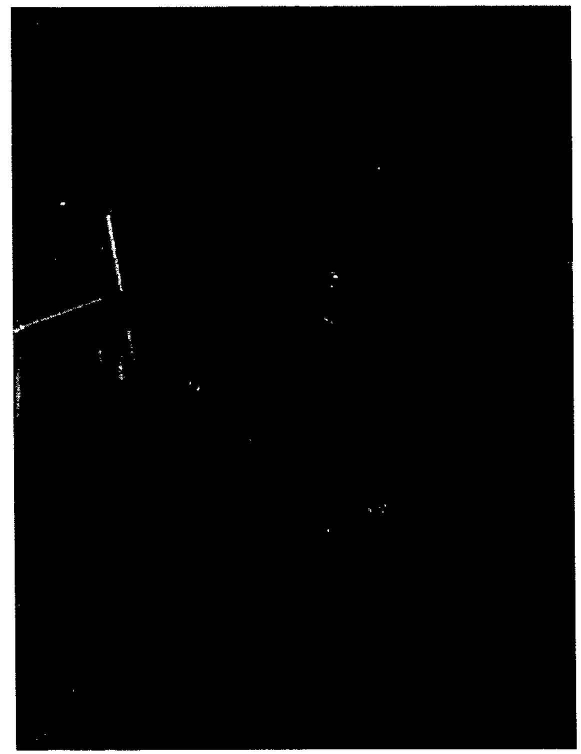
B

Figures 2.3.6.2A and B: Sample fiducials used to align layers

Figures 2.3.6.3

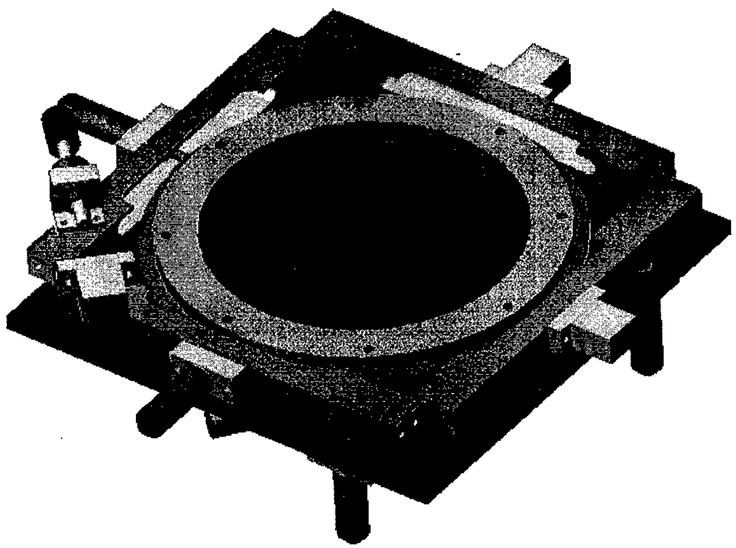


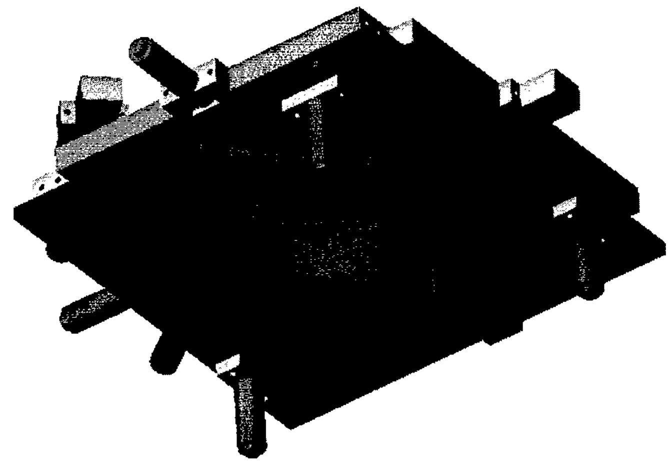




Figures 2.3.6. 3: Alignment tool used for multilayer alignment

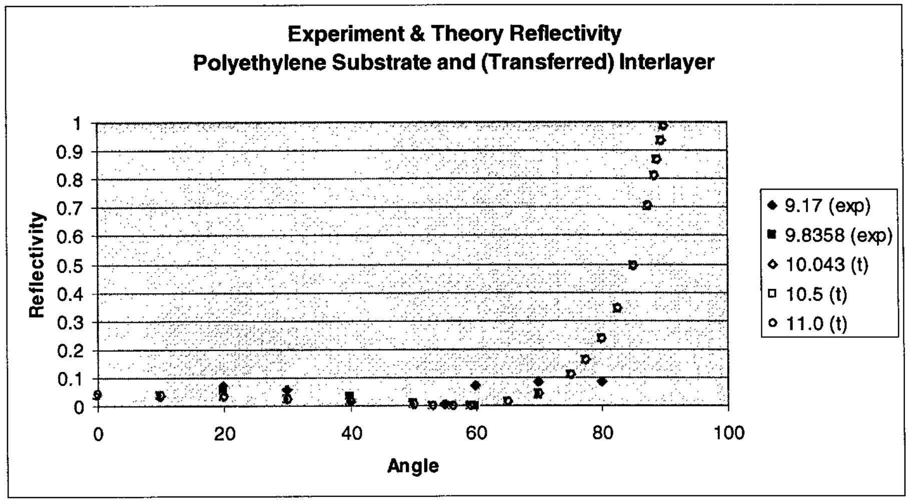
Figures 2.3.6.4





Figures 2.3.6.4 : Alignment Tool Detail

Figures 3.0.1



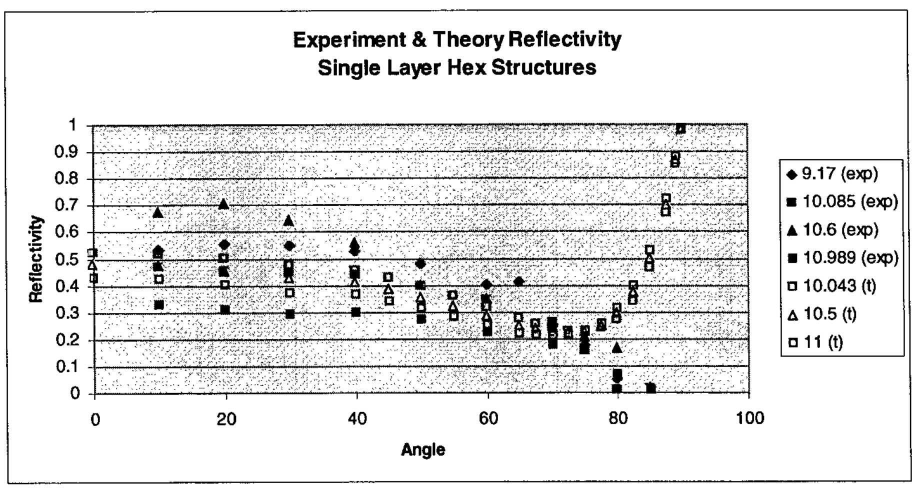
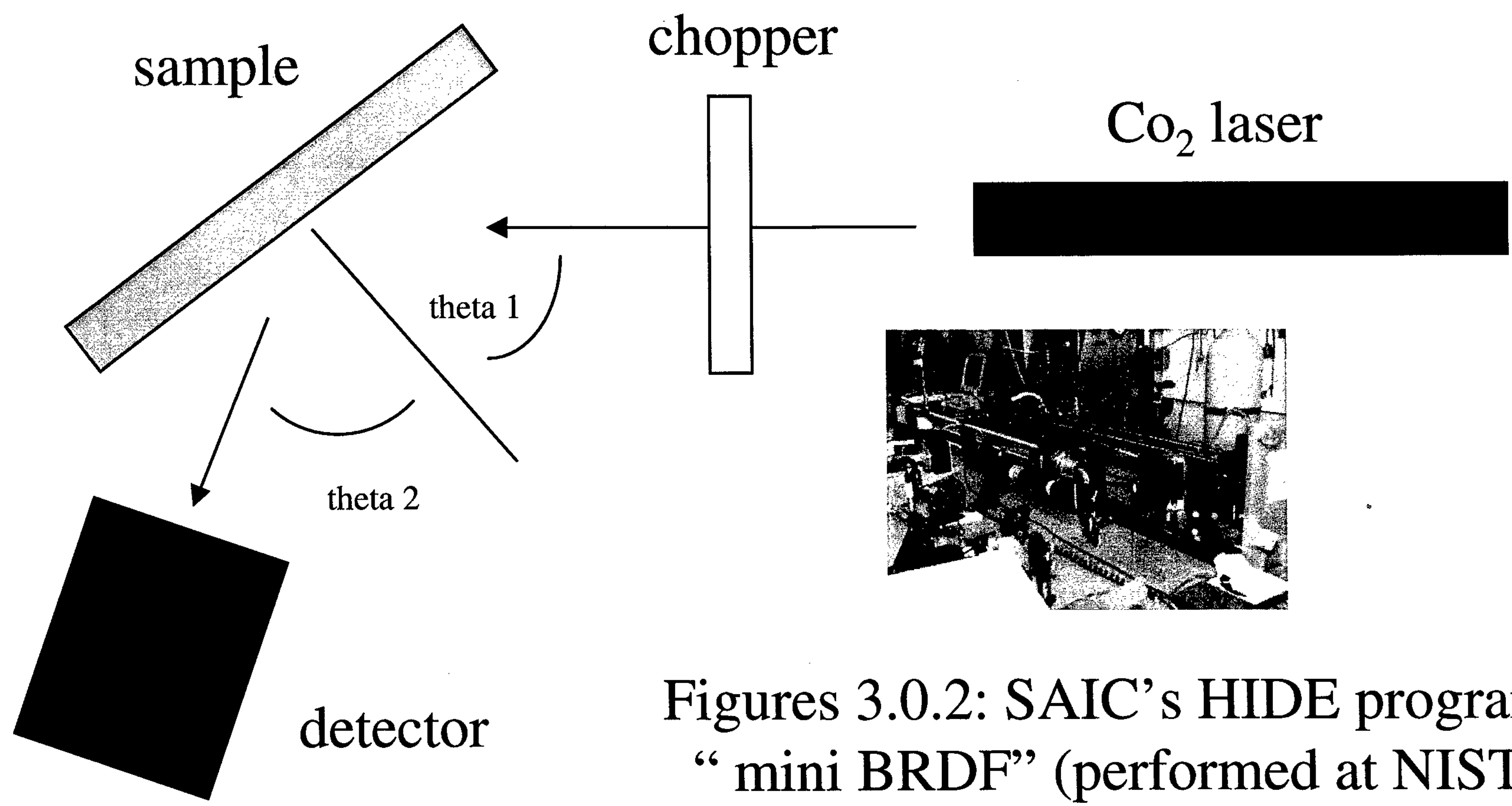


Figure 3.0.1: Experimental results and theoretical predictions for substrate+interlayer and for transferred hex structure

Figures 3.0.2



Figures 3.0.2: SAIC's HIDE program " mini BRDF" (performed at NIST, Boulder)

Reflection and Transmission Coefficients by Periodic Array of Dielectric Spheres in the Spectral Domain

Abstract

A semi-analytic integral equation approach is formulated for the computation of the reflection and transmission coefficients of a periodic single or multilayer array of dielectric or metallic spheres inside a host medium, which may be lossy. It is shown that this method is equivalent to that of applying the boundary conditions at the surface of the spheres, but it has the advantage that it provides an easy transition from the real to the spectral domain, where the convergence of the computed quantities is much faster. In a three dimensional lattice, two methods are presented for computing the dispersion relation of the photonic crystal. The reflection and transmission coefficients are computed for a single or multilayer array of spheres embedded in a slab. Due to the small size of the matrices involved in the computations and the fast convergence, there is a small requirement for computer memory and time.

I. Introduction

In recent years there has been significant progress in the theoretical and experimental investigation of photonic band gap crystals. In most of the work that has been done, simple shapes for the dielectric or metallic materials were chosen such as cylinders with circular or rectangular cross-section for the two-dimensional crystals and spheres or rods with rectangular cross-section for the three-dimensional crystals. The scattering of light by a single layer periodic array of spheres was treated by K. Ohtaka et. al. [1-4], where the analogy between low-energy electron scattering and the light scattering by the dielectric spheres was demonstrated and the connection was made between the reflection of light and its integrated density of states. A formalism for the same problem was developed by A. Modinos [5] by the direct application of the boundary conditions at the surface of the spheres. This formalism was applied in the computation of the reflectivity of a single layer array by N. Stefanou et. al. [6] and in the computation of the transmittance of a multilayer array of the photonic band structure of a three-dimensional array by A. Modinos et. al. [7].

Various techniques have been developed for the computation of the dispersion relation of the photonic crystal such as the plane-wave expansion method [8-12] and the transfer matrix method [13-16]. The former method has been applied for scalar and vector fields. In the vector case, the fields are discontinuous at the boundaries between different dielectrics. Consequently, the truncation of the Fourier series in the spectral domain contains high spectral components, so that convergence becomes a serious problem for the vector fields. For example, R.D. Meade et. al. [11] used 10^6 plane waves to obtain reliable numerical results. Convergence is improved if the sharp edges are smoothed to suppress the high spatial frequencies in the Fourier series. This was done by H.S. Süzüer et. al. [12] to remove the discontinuity of the fields. Even so, the plane wave method is not sufficient for more elaborate photonic crystals such as crystals with defects or containing metal. The transfer matrix method is applied in real space and is fairly easy to implement. It provides for the computation of either the dispersion relation or the reflection and transmission coefficients for crystals of finite size. Due to the large number of mesh points needed for accurate computations, the transfer matrix method may lead to numerically unstable

solutions. Another method that was developed to avoid this problem is the R-matrix propagator method [17]. It was applied to two-dimensional structures to compute both the band structure and the transmission in photonic media.

In this paper, the scattered field and, therefore, the reflection and transmission coefficients for a single layer periodic array of dielectric spheres embedded in a host medium are computed with the help of an integral equation which is known in electromagnetic theory as the Ewald-Oseen extinction theorem [18]. The unknown quantities which are determined by using this theorem are the electric and magnetic currents at the surface of the spheres. Then the fields inside and outside the spheres can be computed from these surface currents. In the integral equation approach presented in this paper, either the electric field by itself or the magnetic field by itself is sufficient for the whole computation of the scattered field. This is not the case when the boundary conditions are applied where both the electric and magnetic tangential components to the surface of the spheres are needed for the computation. The integral equation method is shown to be equivalent to that by A. Modinos [5], but it leads naturally into formulating the problem from the real into the spectral domain. In a lossless host medium, the main advantage of the spectral domain computation is that it provides faster convergence. Thus, in a two-dimensional array, the terms to be summed in the function $Z_{lm}^{l'm'}$ (cf. Section IV) are inversely proportional to the distance of the lattice in the real domain, while they are inversely proportional to the cubic power of the distance in the reciprocal lattice (spectral domain). In a three dimensional array it is even better, since the terms to be summed are still inversely proportional to the distance of the lattice in the real domain, but they are inversely proportional to the fourth power of the distance in the reciprocal lattice. In a lossy host medium, if the loss is fairly large, the computation becomes faster in the real domain due to the exponentially decaying terms present in the expressions for the fields.

In the integral equation approach and in the approach by A. Modinos [5], the fields are expanded in vector spherical harmonics with (l,m) eigennumbers. In Table I in the paper by N. Stefanou [6] it is shown that a maximum value of l_{max}=5 is sufficient for accurate results. The dimension of the matrices involved in the computations is $2l_{max}(l_{max}+2)*2l_{max}(l_{max}+2)$. Thus, with l_{max}=5, the dimension of the matrices is 70x70 which is modest compared to the plane wave method. Consequently, the scattering and transfer matrices, at frequencies where only a few propagating modes are present, are small in size and they should not lead to unstable solutions when multilayer arrays are considered. Another advantage of the integral equation approach, since it is equivalent to that of applying the boundary conditions, is that the discontinuity of the fields at the sharp boundaries (surfaces of the spheres) is built into the solution, which is not the case in the plane-wave method.

In a three-dimensional lattice, two approaches are provided for the computation of the dispersion relation of the photonic crystal (cf. section V), either by setting the determinant of a linear homogeneous algebraic system equal to zero or by applying Bloch's theorem as it was done in the paper by N. Stefanou et. al. [6]. Since the size of the matrices involved is small, the requirement in computer memory is small. Also, from the discussion above, it follows that the computation in the spectral domain should be fast and, therefore, the requirement in computer time is small. The main disadvantage of the method presented in this paper is that it is confined to non-overlapping dielectric or metallic spheres. But the method can be extended to other shapes of scatterers as long as a complete set of functions exists to expand the surface electric and magnetic currents. Thus, the method can be extended to cylinders of circular or rectangular

cross section and to multilayer periodic structures where each layer consists of parallel rods of circular or rectangular cross section.

II. Integral Equation Approach for a Single Sphere

A dielectric sphere is centered at the origin of the coordinate system and has conductivity g_3 and dielectric constant ε_3 (in Mks units). It will be referred as medium 3. Medium 2 outside the sphere has conductivity g_2 and dielectric constant ε_2. We define the complex wavenumbers σ_i, i=2,3 as follows:

$$\sigma_i^2 = j\omega\mu_0(g_i + j\omega\varepsilon_i), \tag{1}$$

where μ_0 is the magnetic permeability of vacuum, ω is the frequency and j is the imaginary unit. Everywhere, in the following, the time-dependence is assumed to be $e^{j\omega t}$. In terms of σ_i, the outward radial Green's functions in the two media are defined by the relations

$$G_i(\mathbf{r}) = \frac{1}{4\pi r} e^{-\sigma_i r}, \tag{2}$$

where $r=|\mathbf{r}|$ and i=2,3.

At the surface of the sphere, we define the electric and magnetic surface currents

$$\mathbf{J}^{(e)}(S) = \left[\mathbf{e}_r \times \mathbf{H}_3(\mathbf{r})\right]_{r=R}, \tag{3a}$$

$$\mathbf{J}^{(m)}(S) = -\left[\mathbf{e}_r \times \mathbf{E}_3(\mathbf{r})\right]_{r=R}, \tag{3b}$$

Here, $\mathbf{E}_3(\mathbf{r})$, $\mathbf{H}_3(\mathbf{r})$ are the electric and magnetic fields inside the sphere, S is a point on the surface S_R of the sphere, determined by the spherical coordinates (R, θ, φ), R is the radius of the sphere and $\mathbf{e}_r$ is the outward unit vector normal to the surface of the sphere.

In the following we shall use the vector spherical harmonics [19] as the complete set to express the angular dependence of vectors on $\Omega_r \equiv(\theta, \varphi)$. Their definition and the relations they satisfy are given in Appendix I. Since $\mathbf{Y}_{lll}^m(\Omega_r)$ is normal to $\mathbf{e}_r$, as well as $\mathbf{e}_r\times \mathbf{Y}_{lll}^m(\Omega_r)$, the most general expression of the electric and magnetic surface currents is as follows:

$$\mathbf{J}^{(e)}(S) = \sum_{lm}\left[I_{lm}^{(M)}\mathbf{Y}_{lll}^m(\Omega_r) - jI_{lm}^{(E)}\mathbf{e}_r \times \mathbf{Y}_{lll}^m\right], \tag{4a}$$

$$\mathbf{J}^{(M)}(S) = \sum_{lm}\left[V_{lm}^{(E)}\mathbf{Y}_{lll}^m(\Omega_r) - jV_{lm}^{(M)}\mathbf{e}_r \times \mathbf{Y}_{lll}^m(\Omega_r)\right], \tag{4b}$$

where the summation extends over l=1,2,3,..., m=-l,-l+1,...,l-1,l. The four sets of unknown coefficients $I_{lm}^{(M)}, I_{lm}^{(E)}, V_{lm}^{(M)}, V_{lm}^{(E)}$ will be determined by solving an integral equation and imposing one of the conditions in Eq. (3a) or Eq. (3b).

Let us define the electric and magnetic vector potentials by means of the surface integrals of the electric and magnetic surface currents, i.e.,

$$\mathbf{A}_i^{(h)}(\mathbf{r}) = \int_{S_r} G_i(\mathbf{r}-\mathbf{r}')\mathbf{J}^{(h)}(S')dS', \tag{5}$$

where h=e,m and i=2,3. In accordance with the paper by E. Wolf [18], we define the electric and magnetic fields for i=2,3 namely,

$$\mathbf{E}_i^{(J)}(\mathbf{r}) = -\frac{j\omega\mu_0}{\sigma_i^2}\nabla\times\nabla\times\mathbf{A}_i^{(e)}(\mathbf{r}) + \nabla\times\mathbf{A}_i^{(m)}(\mathbf{r}), \tag{6a}$$

$$\mathbf{H}_i^{(J)}(\mathbf{r}) = -\frac{1}{j\omega\mu_0}\nabla\times\nabla\times\mathbf{A}_i^{(m)}(\mathbf{r}) - \nabla\times\mathbf{A}_i^{(e)}(\mathbf{r}), \tag{6b}$$

Since

$$\nabla^2\mathbf{A}_i^{(h)}(\mathbf{r}) - \sigma_i^2\mathbf{A}_i^{(h)}(\mathbf{r}) = 0, \tag{7}$$

for all $\mathbf{r}$ except for $\mathbf{r}$ on S_R, an equivalent expression for these fields is:

$$\mathbf{E}_i^{(J)}(\mathbf{r}) = j\omega\mu_0\left[\mathbf{A}_i^{(e)}(\mathbf{r}) - \frac{1}{\sigma_i^2}\nabla(\nabla\cdot\mathbf{A}_i^{(e)}(\mathbf{r})\right] + \nabla\times\mathbf{A}_i^{(m)}(\mathbf{r}), \tag{8a}$$

$$\mathbf{H}_i^{(J)}(\mathbf{r}) = \frac{\sigma_i^2}{j\omega\mu_0}\left[\mathbf{A}_i^{(M)}(\mathbf{r}) - \frac{1}{\sigma_i^2}\nabla\left(\nabla\cdot\mathbf{A}_i^{(m)}(\mathbf{r})\right)\right] - \nabla\times\mathbf{A}_i^{(e)}(\mathbf{r}), \tag{8b}$$

The superscript (J) indicates that $\mathbf{E}_i^{(J)}(\mathbf{r}), \mathbf{H}_i^{(J)}(\mathbf{r})$ depend on $\mathbf{J}^{(e)}(S)$, $\mathbf{J}^{(m)}(S)$ and therefore, they depend on the unknown sets of coefficients $I_{lm}^{(M)}, I_{lm}^{(E)}, V_{lm}^{(M)}, V_{lm}^{(E)}$.

First, we confine ourselves in the region inside the sphere. Substitution of the Green's function as given by Eq. (I11) in Appendix I and the surface currents, as given by Eqs. (4a), 4b), and a rather lengthy but straightforward computation of $\mathbf{E}_i^{(J)}(\mathbf{r}), \mathbf{H}_i^{(J)}(\mathbf{r})$ in Eqs. (6a) and (6b) leads to the following relations:

$$\mathbf{E}_i^{(J)}(\mathbf{r}) = j\sum_{lm}\left[\mathcal{E}_{i,lm}^{(M,in)}\mathbf{E}_{i,lm}^{(M,in)}(\mathbf{r}) + \mathcal{E}_{i,lm}^{(E,in)}\mathbf{E}_{i,lm}^{(E,in)}(\mathbf{r})\right], \tag{9a}$$

$$\mathbf{H}_i^{(J)}(\mathbf{r}) = \frac{\sigma_i}{j\omega\mu_0}\sum_{lm}\left[\mathcal{E}_{i,lm}^{(E,in)}\mathbf{E}_{i,lm}^{(M,in)}(\mathbf{r}) + \mathcal{E}_{i,lm}^{(M,in)}\mathbf{E}_{i,lm}^{(E,in)}(\mathbf{r})\right], \tag{9b}$$

where i=2,3 and

$$\mathbf{E}_{i,lm}^{(M,in)}(\mathbf{r}) = f_l(\sigma_i r)\mathbf{Y}_{lll}^m(\Omega_r)\Theta(R-r), \tag{10a}$$

$$\mathbf{E}_{i,lm}^{(E,in)}(\mathbf{r}) = \frac{1}{j\sigma_i}\nabla\times\left(f_l(\sigma_i\mathbf{r})\mathbf{Y}_{lll}^m(\Omega_r)\right)\Theta(R-r), \tag{10b}$$

The function $\Theta(x)$ is defined as follows:

$$\Theta(x)=\begin{matrix} 1 & x>0, \\ 0 & x<0. \end{matrix} \tag{11}$$

Also:

$$\mathcal{E}_{i,lm}^{(M,in)}=z_i^2\left[\frac{\omega\mu_0}{\sigma_i}g_l(z_i)I_{lm}^{(M)}-\frac{1}{z_i}\left[z_i g_l(z_i)\right]' V_{lm}^{(M)}\right], \tag{12a}$$

$$\mathcal{E}_{i,lm}^{(E,in)}=z_i^2\left[-\frac{\omega\mu_0}{\sigma_i}\frac{1}{z_i}\left[z_i g_l(z_i)\right]' I_{lm}^{(E)}+g_l(z_i)V_{lm}^{(E)}\right], \tag{12b}$$

where $z_i=\sigma_i R$ and

$$\frac{1}{z}\left[z g_l(z)\right]' \equiv g_l'(z)+\frac{1}{z}g_l(z)=-\frac{l}{2l+1}g_{l+1}(z)-\frac{l+1}{2l+1}g_{l-1}(z). \tag{13}$$

The prime indicates differentiation with respect to z. Use was made of Eq. (13) in deriving Eqs. (12a) and (12b).

The fields inside the sphere are given by $\mathbf{E}_3(\mathbf{r})$, $\mathbf{H}_3(\mathbf{r})$. Notice that these fields are not independent of each other, since they satisfy Maxwell's equations. If one of the two fields is known, the other can be computed from the curl of the known field. Next, one of the conditions, given by Eqs. (3a) and (3b) will be imposed on the field at the surface of the sphere. Applying the identities (I5a)-(I5c) in Appendix I, on Eqs. (9a) and (9b) we obtain the relations (we omit the superscript (J) for the fields inside the sphere).

$$\left[\mathbf{e}_r\times\mathbf{E}_3(\mathbf{r})\right]_{r=R}=\sum_{lm}\left[-\mathcal{E}_{3,lm}^{(E,in)}\frac{1}{z_3}\left[z_3 f_l(z_3)\right]'\mathbf{Y}_{lll}^m(\Omega_r)+j\mathcal{E}_{3,lm}^{(M,in)}f_l(z_3)\mathbf{e}_r\times\mathbf{Y}_{lll}^m(\Omega_r)\right], \tag{14a}$$

$$\left[\mathbf{e}_r\times\mathbf{H}_3(\mathbf{r})\right]_{r=R}=\frac{\sigma_3}{\omega\mu_0}\sum_{lm}\left[\mathcal{E}_{3,lm}^{(M,in)}\frac{1}{z_3}\left[z_3 f_l(z_3)\right]'\mathbf{Y}_{lll}^m(\Omega_r)-j\mathcal{E}_{3,lm}^{(E,in)}f_l(z_3)\mathbf{e}_r\times\mathbf{Y}_{lll}^m(\Omega_r)\right], \tag{14b}$$

where use was made of the identity.

$$\frac{1}{z}\left[z f_l(z)\right]' \equiv f_l'(z)+\frac{1}{z}f_l(z)=\frac{l}{2l+1}f_{l+1}(z)+\frac{l+1}{2l+1}f_{l-1}(z), \tag{15}$$

Condition (3a) provides the relations

$$\mathcal{E}_{3,lm}^{(M,in)}\frac{1}{z_3}\left[z_3 f_l(z_3)\right]'=\frac{\omega\mu_0}{\sigma_3}I_{lm}^{(M)}, \tag{16a}$$

$$\mathcal{E}^{(E,in)}_{3,lm} f_l(z_3) = \frac{\omega\mu_0}{\sigma_3} I^{(E)}_{lm}, \tag{16b}$$

while condition (3b) gives the relations:

$$\mathcal{E}^{(M,in)}_{3,lm} f_l(z_3) = V^{(M)}_{lm}, \tag{17a}$$

$$\mathcal{E}^{(E,in)}_{3,lm} \frac{1}{z_3}\left[z_3 f_l(z_3)\right]' = V^{(E)}_{lm}, \tag{17b}$$

where $\mathcal{E}^{(M,in)}_{3,lm}$, $\mathcal{E}^{(E,in)}_{3,lm}$ are given by Eqs. (12a) and (12b) for i=3. If use is made of the identity

$$\frac{1}{z^2} + \frac{1}{z}\left[z g_l(z)\right]' f_l(z) = \frac{1}{z}\left[z f_l(z)\right]' g_l(z), \tag{18}$$

either set of Eqs. (16a), (16b) or Eqs. (17a), (17b) gives the same relations, namely

$$\frac{V^{(M)}_{lm}}{\frac{\omega\mu_0}{\sigma_3} I^{(M)}_{lm}} = \frac{f_l(z_3)}{\frac{1}{z_3}\left[z_3 f_l(z_3)\right]'}, \tag{19a}$$

$$\frac{V^{(E)}_{lm}}{\frac{\omega\mu_0}{\sigma_3} I^{(E)}_{lm}} = \frac{\frac{1}{z_3}\left[z_3 f_l(z_3)\right]'}{f_l(z_3)}. \tag{19b}$$

Thus, the four sets of unknown coefficients have been reduced to two sets. We introduce the two independent sets $A^{(M)}_{lm}$, $A^{(E)}_{lm}$ by means of the relations

$$V^{(M)}_{lm} = f_l(z_3) A^{(M)}_{lm}, \tag{20a}$$

$$I^{(M)}_{lm} = \frac{\sigma_3}{\omega\mu_0} \frac{1}{z_3}\left[z_3 f_3(z_3)\right]' A^{(M)}_{lm}, \tag{20b}$$

$$V^{(E)}_{lm} = \frac{1}{z_3}\left[z_3 f_l(z_3)\right]' A^{(E)}_{lm}, \tag{20c}$$

$$I^{(E)}_{lm} = \frac{\sigma_3}{\omega\mu_0} f_l(z_3) A^{(E)}_{lm}. \tag{20d}$$

Substituting these expressions into Eqs. (12a), (12b). for i=3, and making use of Eq. (18), we obtain the relations

$$\mathcal{E}^{(M,in)}_{3,lm} = A^{(M)}_{lm}, \tag{21a}$$

$$\mathcal{E}_{3,lm}^{(E,in)} = A_{lm}^{(E)}. \tag{21b}$$

On the other hand, for i=2, we obtain the relations

$$\mathcal{E}_{2,lm}^{(M,in)} = -\alpha_l^{(M)} A_{lm}^{(M)}, \tag{22a}$$

$$\mathcal{E}_{2,lm}^{(E,in)} = -\alpha_l^{(E)} A_{lm}^{(E)}, \tag{22b}$$

where

$$\alpha_l^{(M)} = -z_2\left[f_l(z_3)[z_2 g_l(z_2)]' - g_l(z_2)[z_3 f_l(z_3)]'\right], \tag{23a}$$

$$\alpha_l^{(E)} = -z_3\left[f_l(z_3)[z_2 g_l(z_2)]' - \left(\tfrac{z_2}{z_3}\right)^2 g_l(z_2)[z_3 f_l(z_3]'\right]. \tag{23b}$$

Therefore, in terms of the unknown coefficients $A_{lm}^{(M)}, A_{lm}^{(E)}$, the fields inside the sphere are given by the usual expressions

$$\mathbf{E}_3(\mathbf{r}) = j\sum_{lm}\left[A_{lm}^{(M)}\mathbf{E}_{3,lm}^{(M,in)}(\mathbf{r}) + A_{lm}^{(E)}\mathbf{E}_{3,lm}^{(E,in)}(\mathbf{r})\right], \tag{24a}$$

$$\mathbf{H}_3(\mathbf{r}) = \tfrac{\sigma_3}{j\omega\mu_0}\sum_{lm}\left[A_{lm}^{(E)}\mathbf{E}_{3,lm}^{(M,in)}(\mathbf{r}) + A_{lm}^{(M)}\mathbf{E}_{3,lm}^{(E,in)}(\mathbf{r})\right]. \tag{24b}$$

The two sets of unknown coefficients $A_{lm}^{(M)}, A_{lm}^{(E)}$ are determined by an integral equation, which is the Ewald-Oseen Extinction Theorem for the electric field (or for the magnetic field), as stated in the paper by E. Wolf [18]. The theorem states that for all **r** inside the surface S (in our case inside the sphere) the following integral equation is satisfied:

$$\mathbf{E}_2^{(J)}(\mathbf{r}) + \mathbf{E}_2^{(S)}(\mathbf{r}) = 0, \tag{25}$$

where $\mathbf{E}_2^{(J)}(\mathbf{r})$ is given by Eq. (6a) or Eq. (8a) in general and by Eqs. (9a), (22a), (22b), in particular, for the case of the sphere. Therefore, for the sphere, $\mathbf{E}_2^{(J)}(\mathbf{r})$ is equal to

$$\mathbf{E}_2^{(J)}(\mathbf{r}) = -j\sum_{lm}\left[\alpha_l^{(M)} A_{lm}^{(M)}\mathbf{E}_{2,lm}^{(M,in)}(\mathbf{r}) + \alpha_l^{(E)} A_{lm}^{(E)}\mathbf{E}_{2,lm}^{(E,in)}(\mathbf{r})\right]. \tag{26}$$

$\mathbf{E}_2^{(S)}(\mathbf{r})$ is the source (or driver) electric field that originates outside the surface S, i.e., in medium 2.

Similarly, the unknown coefficients $A_{lm}^{(M)}, A_{lm}^{(E)}$ can be determined by the Ewald-Oseen Extinction Theorem for the magnetic field [18], which states that for all **r** inside the surface S, i.e., the sphere, the following integral equation is satisfied:

$$\mathbf{H}_2^{(J)}(\mathbf{r}) + \mathbf{H}_2^{(S)}(\mathbf{r}) = 0, \tag{27}$$

where $\mathbf{H}_2^{(J)}(\mathbf{r})$ is given by Eq. (6b) or Eq. (8b) in general and by Eqs. (9b), (22a), (22b), in particular, for the sphere. Then, for the sphere, $\mathbf{H}_2^{(J)}(\mathbf{r})$ is equal to

$$\mathbf{H}_2^{(J)}(\mathbf{r}) = -\frac{\sigma_2}{j\omega\mu_0}\sum_{l,m}\left[\alpha_l^{(E)} A_{lm}^{(E)} \mathbf{E}_{2,lm}^{(M,in)}(\mathbf{r}) + \alpha_l^{(M)} A_{lm}^{(M)} \mathbf{E}_{2,lm}^{(E,in)}(\mathbf{r})\right]. \tag{28}$$

$\mathbf{H}_2^{(s)}(\mathbf{r})$ is the source magnetic field that originates outside the surface S.

If the source field is a free field in medium 2, then, in the plane wave representation, it is given by the expression

$$\begin{aligned}\mathbf{E}_2^{(S)}(\mathbf{r}) = e^{-jk_\rho\cdot\rho}\Big[&\left(E_{\mathbf{k}}^{(TE+)}(0)e^{-\gamma_2 z} + E_{\mathbf{k}}^{(TE-)}(0)e^{\gamma_2 z}\right)\left(\mathbf{e}_z \times \hat{\mathbf{k}}_\rho\right)\\ &+\left(E_{\mathbf{k}}^{(TM+)}(0)e^{-\gamma_2 z} + E_{\mathbf{k}}^{(TM-)}(0)e^{\gamma_2 z}\right)\hat{\mathbf{k}}_\rho\\ &-\left(E_{\mathbf{k}}^{(TM+)}(0)e^{-\gamma_2 z} - E_{\mathbf{k}}^{(TM-)}(0)e^{\gamma_2 z}\right)\frac{jk_\rho}{\gamma_2}\mathbf{e}_z\Big],\end{aligned} \tag{29a}$$

$$\begin{aligned}\mathbf{H}_2^{(S)}(\mathbf{r}) = \frac{\sigma_2}{j\omega\mu_0}e^{-jk_\rho\cdot\rho}\Big[&-\left(E_{\mathbf{k}}^{(TE+)}(0)e^{-\gamma_2 z} - E_{\mathbf{k}}^{(TE-)}(0)e^{\gamma_2 z}\right)\frac{\gamma_2}{\sigma_2}\hat{\mathbf{k}}_\rho\\ &+\left(E_{\mathbf{k}}^{(TM+)}(0)e^{-\gamma_2 z} - E_{\mathbf{k}}^{(TM-)}(0)e^{\gamma_2 z}\right)\frac{\sigma_2}{\gamma_2}\left(\mathbf{e}_z \times \hat{\mathbf{k}}_\rho\right)\\ &+\left(E_{\mathbf{k}}^{(TE+)}(0)e^{-\gamma_2 z} + E_{\mathbf{k}}^{(TE-)}(0)e^{\gamma_2 z}\right)\frac{jk_\rho}{\sigma_2}\mathbf{e}_z\Big],\end{aligned} \tag{29b}$$

where

$$\gamma_2 = \left[k_\rho^2 + \sigma_2^2\right]^{1/2}. \tag{30}$$

Here, $E_{\mathbf{k}}^{(TE\pm)}(0), E_{\mathbf{k}}^{(TM\pm)}(0)$ are the amplitudes of the electric field at z=0, moving in the forward (+) and backward (–) directions, for the transverse electric (TE) and transverse magnetic (TM) plane waves, respectively. Also, $\mathbf{k}_\rho$ is the projection of the wavevector on the xy-plane, k_ρ is its magnitude and $\hat{\mathbf{k}}_\rho$ is the unit vector in the direction of $\mathbf{k}_\rho$. If (θ_k, φ_k) provide the direction of the plane wavefront with constant phase, in spherical coordinates, then

$$\hat{\mathbf{k}}_\rho = \mathbf{e}_x \cos\varphi_k + \mathbf{e}_y \sin\varphi_k, \tag{31a}$$

$$k_\rho = k\sin\theta_k , \tag{31b}$$

$$\gamma_{2i} = k\cos\theta_k , \tag{31c}$$

where γ_{2i}, is the imaginary part of γ_2 and k is to be determined. If σ_2 is expressed by the complex index of refraction, i.e.,

$$\sigma_2 = (k_2 + jn_2)\tfrac{\omega}{c}, \tag{32}$$

where c is the velocity of light in vacuum, then, k can be computed with the help of Eqs. (30), (31b), (31c) and k_ρ becomes equal to

$$k_\rho = \sqrt{n_2^2 - k_2^2}\,\tfrac{\omega}{c}\sin\theta_k\left[\tfrac{1}{2}\left(1+\sqrt{1+\left(\frac{2k_2n_2}{\left(n_2^2-k_2^2\right)\cos\theta_k}\right)^2}\right)\right]^{1/2} . \tag{33}$$

For simplicity, we assumed that $k_2<n_2$ which is usually the case.

If use is made of Eq. (II 19) in Appendix II and of the orthonormality of the scalar spherical harmonics, then, the source field, in the spherical wave representation becomes equal to

$$\mathbf{E}_2^{(S)}(\mathbf{r}) = j\sum_{lm}\left[A_{lm}^{(MS)}f_l(\sigma_2 r)\mathbf{Y}_{lll}^{m}(\Omega_r) + A_{lm}^{(ES)}\tfrac{1}{j\sigma_2}\nabla\times\left(f_l(\sigma_2 r)\mathbf{Y}_{lll}^{m}(\Omega_r)\right)\right] , \tag{34a}$$

$$\mathbf{H}_2^{(S)}(\mathbf{r}) = \tfrac{\sigma_2}{j\omega\mu_0}\sum_{lm}\left[A_{lm}^{(ES)}f_l(\sigma_2 r)\mathbf{Y}_{lll}^{m}(\Omega_r) + A_{lm}^{(MS)}\tfrac{1}{j\sigma_2}\nabla\times\left(f_l(\sigma_2 r)\mathbf{Y}_{lll}^{m}(\Omega_r)\right)\right] , \tag{34b}$$

where

$$\begin{aligned} A_{lm}^{(MS)} &= -\frac{4\pi j}{[l(l+1)]^{1/2}}(-1)^{l-m+l} \\ &* \Big\{\tilde{C}_{lm}^{(TE)}\left[E_{\mathbf{k}}^{(TE+)}(0) + (-1)^{l-m+l}E_{\mathbf{k}}^{(TE-)}(0)\right] \\ &+ \left(\tfrac{\sigma_2}{\gamma_2}\right)^2\tilde{C}_{lm}^{(TM)}\left[E_{\mathbf{k}}^{(TM+)}(0) + (-1)^{l-m+l}E_{\mathbf{k}}^{(TM-)}(0)\right]\Big\}, \end{aligned} \tag{35a}$$

$$\begin{aligned} A_{lm}^{(ES)} &= -\frac{4\pi}{[l(l+1)]^{1/2}}\frac{\sigma_2}{\gamma_2}(-1)^{l-m+l} \\ &* \Big\{\tilde{C}_{lm}^{(TM)}\left[E_{\mathbf{k}}^{(TE+)}(0) + (-1)^{l-m+l}E_{\mathbf{k}}^{(TE-)}(0)\right] \\ &- \tilde{C}_{lm}^{(TE)}\left[E_{\mathbf{k}}^{(TM+)}(0) + (-1)^{l-m+l}E_{\mathbf{k}}^{(TM-)}(0)\right]\Big\}, \end{aligned} \tag{35b}$$

and

$$\widetilde{C}_{lm}^{(TM)} = \alpha_l^m \widetilde{Y}_{l,-m-1}\left(\frac{\gamma_2}{\sigma_2}, \varphi_k\right) e^{j\varphi_k} + \beta_l^m \widetilde{Y}_{l,-m+1}\left(\frac{\gamma_2}{\sigma_2}, \varphi_k\right) e^{-j\varphi_k} , \tag{36a}$$

$$\widetilde{C}_{lm}^{(TE)} = j\left[\alpha_l^m \widetilde{Y}_{l,-m-1}\left(\frac{\gamma_2}{\sigma_2}, \varphi_k\right) e^{j\varphi_k} - \beta_l^m \widetilde{Y}_{l,-m+1}\left(\frac{\gamma_2}{\sigma_2}, \varphi_k\right) e^{-j\varphi_k}\right] \tag{36b}$$

$$\alpha_l^m = \tfrac{1}{2}\left[(l-m)(l+m+1)\right]^{1/2} , \tag{37a}$$

$$\beta_l^m = \tfrac{1}{2}\left[(l+m)(l-m+1)\right]^{1/2} . \tag{37b}$$

The complex scalar spherical harmonics $\widetilde{Y}_{lm}\left(\frac{\gamma_2}{\sigma_2}, \varphi_k\right)$ have been defined in Appendix II, Eq. (II 19). When medium 2 is non-absorptive, i.e., σ_2 is purely imaginary, they reduce to the usual scalar spherical harmonics.

Substitution of the source electric field in the spherical wave representation, into Eq. (25) determines the unknown coefficients $A_{lm}^{(M)}, A_{lm}^{(E)}$, namely,

$$A_{lm}^{(M)} = \frac{1}{\alpha_l^{(M)}} A_{lm}^{(MS)} , \tag{38a}$$

$$A_{lm}^{(E)} = \frac{1}{\alpha_l^{(E)}} A_{lm}^{(ES)} , \tag{38b}$$

where use was made of the orthonormality property of the vector spherical harmonics. These are the same expressions obtained by the application of the boundary conditions at r=R, i.e., continuity of the tangential components of the electric and magnetic field. Notice that the application of the Ewald-Oseen extinction theorem led to the determination of the unknown coefficients $A_{lm}^{(M)}, A_{lm}^{(E)}$ without any reference to the fields outside the sphere. Also, once the electric and magnetic surface currents were expanded in terms of a complete set, one of the boundary conditions, i.e., either Eq. (3a) or Eq. (3b) was indispensable in reducing the four sets of unknown coefficients $V_{lm}^{(M)}$, $V_{lm}^{(E)}$, $I_{lm}^{(M)}$, $I_{lm}^{(E)}$ into two sets. The same result, i.e., Eqs. (38a), (38b) would have been obtained if the Ewald-Oseen extinction theorem for the magnetic field was applied.

Therefore, in general, it is possible to determine the fields in a dielectric medium 3 which lies inside medium 2 with their boundary being the surface S and the source field originating outside medium 3. For this purpose, the electric and magnetic surface currents on S are expanded in terms of a complete set of functions with four unknown sets of coefficients. If use is made only of the electric field inside S, then the boundary condition, Eq. (36), is imposed which provides two linear algebraic sets of equations for the four unknown sets of coefficients, by making use of the orthonormality property of the complete set. Two more linear algebraic sets of equations are provided by the integral equation (25). These four sets of linear algebraic equations with four unknown sets of coefficients determine the electric field inside S. The magnetic field inside S is computed from the curl of the electric field. On the other hand, if use is made only of the

magnetic field inside S, then the boundary condition, Eq. (3a), together with the integral equation (27) determine the magnetic field inside S. The electric field is computed from the curl of the magnetic field.

Next, we consider the scattered field outside the sphere S. Substitution of the Green's function, i.e., Eq. (I 11) and the surface currents, i.e., Eqs. (4a), (4b), into Eqs. (6a), (6b) for i=2, leads to the relations

$$\mathbf{E}_2^{(sc)}(\mathbf{r}) = j\sum_{lm}\left[\mathcal{E}_{2,lm}^{(M,out)}\mathbf{E}_{2,lm}^{(M,out)}(\mathbf{r}) + \mathcal{E}_{2,lm}^{(E,out)}\mathbf{E}_{2,lm}^{(E,out)}(\mathbf{r})\right], \tag{39a}$$

$$\mathbf{H}_2^{(sc)}(\mathbf{r}) = \frac{\sigma_2}{j\omega\mu_0}\sum_{lm}\left[\mathcal{E}_{2,lm}^{(E,out)}\mathbf{E}_{2,lm}^{(M,out)}(\mathbf{r}) + \mathcal{E}_{2,lm}^{(M,out)}\mathbf{E}_{2,lm}^{(E,out)}(\mathbf{r})\right], \tag{39b}$$

where

$$\mathbf{E}_{2,lm}^{(M,out)}(\mathbf{r}) = g_l(\sigma_2 r)\mathbf{Y}_{lll}^{M}(\Omega_r)\Theta(r-R), \tag{40a}$$

$$\mathbf{E}_{2,lm}^{(E,out)}(\mathbf{r}) = \frac{1}{j\sigma_2}\nabla\times\left(g_l(\sigma_2 r)\mathbf{Y}_{lll}^{M}(\Omega_r)\right)\Theta(r-R), \tag{40b}$$

Also:

$$\mathcal{E}_{2,lm}^{(M,out)} = -z_2^2\left[\frac{\omega\mu_0}{\sigma_2}f_l(z_2)I_{lm}^{(M)} - \frac{1}{z_2}\left[z_2 f_l(z_2\right]' V_{lm}^{(M)}\right], \tag{41a}$$

$$E_{2,lm}^{(E,out)} = -z_2^2\left[-\frac{\omega\mu_0}{\sigma_2}\frac{1}{z_2}\left[z_2 f_l(z_2)\right]' I_{lm}^{(E)} + f_l(z_2)V_{lm}^{(E)}\right]. \tag{41b}$$

We have renamed the fields to indicate that they are the scattered fields. Replacing $I_{lm}^{(M)}$, $V_{lm}^{(M)}$, $I_{lm}^{(E)}$, $V_{lm}^{(E)}$ from Eqs. (20a) – (20d) into the relations above, we obtain

$$\mathcal{E}_{2,lm}^{(M,out)} = \beta_l^{(M)}A_{lm}^{(M)}, \tag{42a}$$

$$\mathcal{E}_{2,lm}^{(E,out)} = \beta_l^{(E)}A_{lm}^{(E)}, \tag{42b}$$

where

$$\beta_l^{(M)} = z_2\left[f_l(z_3)\left[z_2 f_l(z_2)\right]' - f_l(z_2)\left[z_3 f_l(z_3)\right]'\right], \tag{43a}$$

$$\beta_l^{(E)} = z_3\left[f_l(z_3)\left[z_2 f_l(z_2)\right]' - \left(\frac{z_2}{z_3}\right)^2 f_l(z_2)\left[z_3 f_l(z_3)\right]'\right]. \tag{43b}$$

The total field outside the sphere is equal to

$$\mathbf{E}_2(\mathbf{r}) = \mathbf{E}_2^{(s)}(\mathbf{r}) + \mathbf{E}_2^{(sc)}(\mathbf{r}), \tag{44a}$$

$$\mathbf{H}_2(\mathbf{r}) = \mathbf{H}_2^{(s)}(\mathbf{r}) + \mathbf{H}_2^{(sc)}(\mathbf{r}). \tag{44b}$$

When the source field is a free field, as given by Eqs. (29a), (29b), then, with the help of Eqs. (38a), (38b), (42a), (42b), the scattered field due to the surface currents becomes equal to

$$\mathbf{E}_2^{(sc)}(\mathbf{r}) = j\sum_{l,m}\left[B_{lm}^{(M)}\mathbf{E}_{2,lm}^{(M,out)}(\mathbf{r}) + B_{lm}^{(E)}\mathbf{E}_{2,lm}^{(E,out)}(\mathbf{r})\right] \tag{45a}$$

$$\mathbf{H}_2^{(sc)}(\mathbf{r}) = \frac{\sigma_2}{j\omega\mu_0}\sum_{l,m}\left[B_{lm}^{(E)}\mathbf{E}_{2,lm}^{(M,out)}(\mathbf{r}) + B_{lm}^{(M)}\mathbf{E}_{2,lm}^{(E,out)}(\mathbf{r})\right] \tag{45b}$$

where

$$B_{lm}^{(M)} = \frac{\beta_l^{(M)}}{\alpha_l^{(M)}}A_{lm}^{(MS)}, \tag{46a}$$

$$B_{lm}^{(E)} = \frac{\beta_l^{(E)}}{\alpha_l^{(E)}}A_{lm}^{(ES)}. \tag{46b}$$

These are the same expressions obtained by applying the boundary conditions at the surface of the sphere. Therefore, the integral equation approach provides the correct solution inside and outside the sphere. In the general case of any surface S, the difficulty of the formalism presented lies in the choice of the complete set to expand the electric and magnetic surface currents. In the case of the sphere, the obvious choice is the vector spherical harmonics, which led to a trivial solution for the linear algebraic set of equations. As we will see in the next section, this is not the case for a two-dimensional periodic array of dielectric spheres embedded in a host medium.

III. Integral Equation Approach for an Array of Spheres

A single layer periodic array of dielectric spheres with conductivity g_3 and dielectric constant ε_3 (medium 3) is embedded in the host medium 2. The unit call in the lattice is determined by the translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$ so that the points in the lattice are given by the relation

$$\mathbf{a}_{pq} = p\mathbf{a}_1 + q\mathbf{a}_2, \tag{47}$$

where p, q are integers. The fundamental vectors of the reciprocal lattice are:

$$\mathbf{B}_1 = 2\pi\frac{\mathbf{a}_2\times\mathbf{e}_z}{\mathbf{a}_1(\mathbf{a}_2\times\mathbf{e}_z)}, \tag{48a}$$

$$\mathbf{B}_2 = 2\pi\frac{\mathbf{e}_z\times\mathbf{a}_1}{\mathbf{a}_1(\mathbf{a}_2\times\mathbf{e}_z)}, \tag{48b}$$

and the points in the reciprocal lattice are given by the relation

$$\mathbf{b}_{pq} = p\mathbf{B}_1 + q\mathbf{B}_2 . \tag{49}$$

The dielectric spheres are centered at $\mathbf{a}_{pq}$ and they do not overlap. At the surface S_{sph} of each sphere there is an electric and magnetic surface current. Due to the periodicity of the system Floquet's theorem applies, and therefore, the electric and magnetic surface current due to all the spheres, centered at $\mathbf{a}_{pq}$, are equal to

$$\mathbf{J}^{(e)}(\mathbf{r}) = \sum_{pq} e^{-j\boldsymbol{\beta}\cdot\mathbf{a}_{pq}} U\left(\left|\mathbf{r}-\mathbf{a}_{pq}\right| \varepsilon S_{sph}\right) \sum_{lm}\left[I_{lm}^{(M)}\mathbf{Y}_{lll}^{m}(\Omega_{r_{pq}}) - jI_{lm}^{(E)}\mathbf{e}_{r_{pq}} \times \mathbf{Y}_{lll}^{m}(\Omega_{r_{pq}})\right] \tag{50a}$$

$$\mathbf{J}^{(M)}(\mathbf{r}) = \sum_{pq} e^{-j\boldsymbol{\beta}\cdot\mathbf{a}_{pq}} U\left(\left|\mathbf{r}-\mathbf{a}_{pq}\right| \varepsilon S_{sph}\right) * \sum_{lm}^{pq}\left[V_{lm}^{(E)}\mathbf{Y}_{lll}^{m}(\Omega_{r_{pq}}) - jV_{lm}^{(M)}\mathbf{e}_{r_{pq}} \times \mathbf{Y}_{lll}^{m}(\Omega_{r_{pq}})\right] \tag{50b}$$

Here, $\boldsymbol{\beta}$ is the phase vector mentioned above, $\Omega_{r_{pq}} = (\theta_{pq}, \varphi_{pq})$, where $(r_{pq}, \theta_{pq}, \varphi_{pq})$ are the spherical coordinates of the vector $\mathbf{r}_{pq} = \mathbf{r} - \mathbf{a}_{pq}$, and

$$U\left(\left|\mathbf{r}-\mathbf{a}_{pq}\right| \varepsilon S_{sph}\right) = \begin{matrix} 1 & \text{if } |\mathbf{r}-\mathbf{a}_{pq}| = R \\ 0 & \text{otherwise} \end{matrix} \tag{51}$$

The surface current on each sphere satisfies the conditions given by Eqs. (3a) or (3b). Using one of these conditions, and following the same procedure as in Section II, we conclude that Eqs. (20a) – (20d) are valid, as well as, Eqs. (21a), (21b) and Eqs. (22a), (22b). Therefore, the fields inside the sphere centered at $\mathbf{a}_{pq}$, i.e., when $|\mathbf{r}-\mathbf{a}_{pq}|<R$, is given by Eqs. (24a), (24b), where $\mathbf{r}$ should be replaced by $\mathbf{r}_{pq}$. On the other hand, when $|\mathbf{r}-\mathbf{a}_{pq}|<R$ in the computation of $\mathbf{E}_2^{(J)}(\mathbf{r})$, $\mathbf{H}_2^{(J)}(\mathbf{r})$, the field due to the sphere centered at $\mathbf{a}_{pq}$ is computed inside that sphere, while for all the other spheres, the field due to them is computed outside these spheres. Taking into account Eqs. (42a), (42b), we conclude that

$$\begin{aligned}\mathbf{E}_2^{(J)}(\mathbf{r}) &= -je^{-j\boldsymbol{\beta}\cdot\mathbf{a}_{pq}} \\ &* \sum_{lm}\Bigg[A_{lm}^{(M)}\left(\alpha_l^{(M)}\mathbf{E}_{2,lm}^{(M,in)}\left(\mathbf{r}_{pq}\right) - \beta_l^{(M)}\sum_{p'q'}{}' e^{-j\boldsymbol{\beta}\cdot\hat{\mathbf{a}}_{p'q'}}\mathbf{E}_{2,lm}^{(M,out)}\left(\mathbf{r}_{pq}-\hat{\mathbf{a}}_{p'q'}\right)\right) \\ &+ A_{lm}^{(E)}\left(\alpha_l^{(E)}\mathbf{E}_{2,lm}^{(E,in)}(\mathbf{r}_{pq}) - \beta_l^{(E)}\sum_{p'q'}{}' e^{-j\boldsymbol{\beta}\cdot\hat{\mathbf{a}}_{p'q'}}\mathbf{E}_{2,lm}^{(E,out)}(\mathbf{r}_{pq}-\hat{\mathbf{a}}_{p'q'})\right)\Bigg]\end{aligned} \tag{52a}$$

$$\mathbf{H}_2^{(J)}(\mathbf{r}) = -\frac{\sigma_2}{j\omega\mu_0} e^{-j\beta\cdot\mathbf{a}_{pq}}$$

$$* \sum_{lm}\left[A_{lm}^{(E)}\left(\alpha_l^{(E)} \mathbf{E}_{2,lm}^{(M,in)}(\mathbf{r}_{pq}) - \beta_l^{(E)} \sum_{p'q'}{}' e^{-j\beta\cdot\hat{\mathbf{a}}_{p'q'}} \mathbf{E}_{2,lm}^{(M,out)}(\mathbf{r}_{pq} - \hat{\mathbf{a}}_{p'q'}) \right)\right. \tag{52b}$$

$$\left. + A_{lm}^{(M)}\left(\alpha_l^{(M)} \mathbf{E}_{2,lm}^{(E,in)}(\mathbf{r}_{pq}) - \beta_l^{(M)} \sum_{p'q'}{}' e^{-j\beta\cdot\hat{\mathbf{a}}_{p'q'}} \mathbf{E}_{2,lm}^{(E,out)}(\mathbf{r}_{pq} - \hat{\mathbf{a}}_{p'q'}) \right)\right]$$

where $\hat{\mathbf{a}}_{p'q'} = \mathbf{a}_{p'q'} - \mathbf{a}_{pq}$. The prime in the summations above means that they extend over all spheres except for the one centered at $\mathbf{a}_{pq}$. The (in) and (out) fields in the relations above have already been defined in the previous section.

Multiplication of Eqs. (52a), (52b) by $\mathbf{E}_{2,lm}^{(M,in)^*}(\mathbf{r}_{pq})$ and integration over the volume V_{pq} of the sphere centered at $\mathbf{a}_{pq}$ yields the following relations:

$$\int_{V_{pq}} \mathbf{E}_2^{(J)}(\mathbf{r}) \cdot \mathbf{E}_{2,lm}^{(M,in)^*}(\mathbf{r}_{pq}) d^3x_{pq} = -je^{-j\beta\cdot\mathbf{a}_{pq}}$$

$$* \sum_{l'm'} \zeta_l \left\{ \left[\frac{\alpha_l^{(M)}}{\beta_l^{(M)}} \delta_{ll'}\delta_{mm'} - \Omega_{lm;l'm'}^{(1)}(\beta) \right] B_{l'm'}^{(M)} - \Omega_{lm;l'm'}^{(2)}(\beta) B_{l'm'}^{(E)} \right\}, \tag{53a}$$

$$\int_{V_{pq}} \mathbf{H}_2^{(J)}(\mathbf{r}) \cdot \mathbf{E}_{2,lm}^{(M,in)^*}(\mathbf{r}_{pq}) d^3x_{pq} = -\frac{\sigma_2}{j\omega\mu_0} e^{-j\beta\cdot\mathbf{a}_{pq}}$$

$$* \sum_{l'm'} \zeta_l \left\{ -\Omega_{lm;l'm'}^{(1)}(\beta) B_{l'm'}^{(M)} + \left[\frac{\alpha_l^{(E)}}{\beta_l^{(E)}} \delta_{ll'}\delta_{mm'} - \Omega_{lm;l'm'}^{(2)}(\beta) \right] B_{l'm'}^{(E)} \right\} \tag{53b}$$

where

$$\Omega_{lm;l'm'}^{(1)}(\beta) = \frac{1}{\zeta_l} \sum_{p'q'} e^{-j\beta\cdot\hat{\mathbf{a}}_{p'q'}} U_{l'm';lm}(\hat{\mathbf{a}}_{p'q'}) \tag{54c}$$

$$\Omega_{lm;l'm'}^{(2)}(\beta) = \frac{1}{\zeta_l} \sum_{p'q'} e^{-j\beta\cdot\hat{\mathbf{a}}_{p'q'}} U_{l'm';lm}(\hat{\mathbf{a}}_{p'q'}), \tag{54d}$$

$$U_{lm;l'm'}(\mathbf{r}_0)\ \int_{V_0}\mathbf{E}_{2,lm}^{(M,out)}(\mathbf{r}-\mathbf{r}_0)\cdot\mathbf{E}_{2,l'm'}^{(M,in)^*}(\mathbf{r})d^3x\,, \tag{55a}$$

$$V_{lm;l'm'}(\mathbf{r}_0)=\int_{V_0}\mathbf{E}_{2,lm}^{(E,out)}(\mathbf{r}-\mathbf{r}_0)\cdot\mathbf{E}_{2,l'm'}^{(M,in)^*}(\mathbf{r})d^3x\,. \tag{55b}$$

$$\zeta_l=\int_0^R|f_l(\sigma_2 r)|^2\,r^2dr=\frac{R^3}{z_2^2-z_2^{*2}}\left[z_2f_{l-1}(z_2)f_l(z_2^*)-z_2^*f_{l-1}(z_2^*)f_l(z_{2)}\right]. \tag{56}$$

Here, we have replaced the unknown coefficients $A_{lm}^{(M)},A_{lm}^{(E)}$ by $B_{lm}^{(M)}=\beta_{lm}^{(M)}A_{lm}^{(M)}$ $B_{lm}^{(E)}=\beta_l^{(E)}A_{lm}^{(E)}$, since the latter provide the scattering properties of the array in which we are interested. Also, δ_{mn} is the Kronecker delta, i.e., $\delta_{mn}=1$, when m=n and zero otherwise.

In the presence of the lattice, the source field's wavevector is not limited, in general, to the wavevector $\mathbf{k}_\rho$ of the incident field. Free fields with wavevectors $\mathbf{K}_{pq}=\mathbf{k}_\rho+\mathbf{b}_{pq}$ where $\mathbf{b}_{pq}$ is a point in the reciprocal lattice (Eq. (49)), could also drive the array of spheres. As we shall see, this is the case at high frequencies, where there can be more than a single angle that the field scatters. Thus, Eqs. (29a), (29b) for the source field should be replaced by the relations:

$$\begin{aligned}\mathbf{E}_2^{(S)}(\mathbf{r})&=\sum_{\mathbf{K}}e^{-j\mathbf{K}\cdot\rho-\gamma_2R}\\&*\Big\{\left[E_{\mathbf{K}}^{(TE+)}(-R)e^{-\gamma_2z}+E_{\mathbf{K}}^{(TE-)}(R)e^{\gamma_2z}\right](\mathbf{e}_z\times\hat{\mathbf{K}})\\&+\left[E_{\mathbf{K}}^{(TM+)}(-R)e^{-\gamma_2z}+E_{\mathbf{K}}^{(TM-)}(R)e^{\gamma_2z}\right]\hat{\mathbf{K}}\\&-\left[E_{\mathbf{K}}^{(TM+)}(-R)e^{-\gamma_2z}-E_{\mathbf{K}}^{(TM-)}(R)e^{\gamma_2z}\right]\frac{jK}{\gamma_2}\mathbf{e}_z\Big\}\end{aligned} \tag{57a}$$

$$\begin{aligned}\mathbf{H}_2^{(S)}(\mathbf{r})&=\frac{\sigma_2}{j\omega\mu_0}\sum_{\mathbf{K}}e^{-j\mathbf{K}\cdot\rho-\gamma_2R}\Big\{-\left[E_{\mathbf{K}}^{(TE+)}(-R)e^{-\gamma_2z}-E_{\mathbf{K}}^{(TE-)}(R)e^{\gamma_2z}\right]\frac{\gamma_2}{\sigma_2}\hat{\mathbf{K}}\\&+\left[E_{\mathbf{K}}^{(TM+)}(-R)e^{-\gamma_2z}-E_{\mathbf{K}}^{(TM-)}(R)e^{\gamma_2z}\right]\frac{\sigma_2}{\gamma_2}(\mathbf{e}_z\times\hat{\mathbf{K}})\\&+\left[E_{\mathbf{K}}^{(TE+)}(-R)e^{-\gamma_2z}+E_{\mathbf{K}}^{(TE-)}(R)e^{\gamma_2z}\right]\frac{jK}{\sigma_2}\mathbf{e}_z\Big\},\end{aligned} \tag{57b}$$

where

$$\gamma_2=\left[\mathbf{K}^2+\sigma_2^2\right]^{1/2}, \tag{58}$$

We have omitted the subscripts p,q in $\mathbf{K}_{pq}=\mathbf{k}_\rho+\mathbf{b}_{pq}$ to simplify the notation. Here, $\hat{\mathbf{K}}$ is the unit vector of $\mathbf{K}$ and K is its magnitude. Also, the amplitudes of the source field are given at z=R and Z=-R, since our aim is to compute the scattering matrix in relation to the planes at z=-R and z=R.

The source field above is in the plane wave representation. In the spherical wave representation, for each wavevector **K**, the source field can be writen as follows (cf. Eq. (II19) and Eqs. (34a), (34b))

$$\mathbf{E}^{(S)}_{2,\mathbf{K}}(\mathbf{r}) = \sum_{st} e^{-j\mathbf{K}\cdot\mathbf{a}_{st}} j\sum_{lm}\Big[A^{(MS)}_{lm}(\mathbf{K}) f_l(\sigma_2 r_{st}) \mathbf{Y}^m_{lll}(\Omega_{r_{st}}) + A^{(ES)}_{lm}(\mathbf{K}) \frac{1}{j\sigma_2} \nabla\times\left(f_l(\sigma_2 r_{st}) \mathbf{Y}^m_{lll}(\Omega_{r_{st}})\right)\Big], \tag{59a}$$

$$\mathbf{H}^{(S)}_{2,\mathbf{K}}(\mathbf{r}) = \frac{\sigma_2}{j\omega\mu_0} \sum_{st} e^{-j\mathbf{K}\cdot\mathbf{a}_{st}} \sum_{lm}\Big[A^{(ES)}_{lm}(\mathbf{K}) f_l(\sigma_2 r_{st}) \mathbf{Y}^m_{lll}(\Omega_{r_{st}}) + A^{(MS)}_{lm}(\mathbf{K}) \frac{1}{j\sigma_2} \nabla\times\left(f_l(\sigma_2 r_{st}) \mathbf{Y}^m_{lll}(\Omega_{r_{st}})\right)\Big], \tag{59b}$$

where

$$A^{(MS)}_{lm}(\mathbf{K}) = -\frac{4\pi j}{[l(l+1)]^{1/2}} e^{-\gamma_2 R}(-1)^{l-m+l} * \Big\{\tilde{C}^{(TE)}_{lm}\left[E^{(TE+)}_{\mathbf{K}}(-R) + (-1)^{l-m+l} E^{(TE-)}_{\mathbf{K}}(R)\right] + \left(\frac{\sigma_2}{\gamma_2}\right)^2 \tilde{C}^{(TM)}_{lm}\left[E^{(TM+)}_{\mathbf{K}}(-R) + (-1)^{l-m+l} E^{(TM-)}_{\mathbf{K}}(R)\right]\Big\}, \tag{60a}$$

$$A^{(ES)}_{lm}(\mathbf{K}) = -\frac{4\pi}{[l(l+1)]^{1/2}} \frac{\sigma_2}{\gamma_2} e^{-\gamma_2 R}(-1)^{l-m+l} * \Big\{\tilde{C}^{(TM)}_{lm}\left[E^{(TE+)}_{\mathbf{K}}(-R) + (-1)^{l-m+l} E^{(TE-)}_{\mathbf{K}}(R)\right] - \tilde{C}^{(TE)}_{lm}\left[E^{(TM+)}_{\mathbf{K}}(-R) + (-1)^{l-m+l} E^{(TM-)}_{\mathbf{K}}(R)\right]\Big\}. \tag{60b}$$

$\tilde{C}^{(TM)}_{lm}$, $\tilde{C}^{(TE)}_{lm}$ are given by Eqs. (36a), (36b), where **k** is replaced by **K**, i.e., $\varphi_{\mathbf{K}}$ is the azimuthal angle of **K**, and γ_2 is given by Eq. (58) Since $\mathbf{b}_{pq}\cdot\mathbf{a}_{st}$ is an integral multiple of 2π, $\exp(-j\mathbf{K}\cdot\mathbf{a}_{st})$ can be replaced by $\exp(-j\mathbf{k}_\rho\cdot\mathbf{a}_{st})$ in Eqs. (59a), (59b).

For each wavevector **K**, multiplication of Eqs. (59a), (59b) by $E^{(M,in)^*}_{2,lm}(\mathbf{r}_{pq})$ and integration over the volume V_{pq} of the sphere centered at $\mathbf{a}_{pq}$ yields the following relation

$$\int_{V_{pq}} \mathbf{E}^{(S)}_{2,K}(\mathbf{r}) \cdot \mathbf{E}^{(M,in)^*}_{2,lm}(\mathbf{r}_{pq}) d^3x_{pq} = je^{-j\mathbf{k}_\rho\cdot\mathbf{a}_{pq}} A^{(MS)}_{lm}(\mathbf{K})\zeta_l, \tag{61a}$$

$$\int_{V_{pq}} \mathbf{H}^{(S)}_{2,\mathbf{K}}(\mathbf{r}) \cdot \mathbf{E}^{(M,in)^*}_{2,lm}(\mathbf{r}_{pq}) d^3x_{pq} = \frac{\sigma_2}{j\omega\mu_0} e^{-j\mathbf{k}_\rho \cdot \mathbf{a}_{pq}} A^{(ES)}_{lm}(\mathbf{K})\zeta_l. \tag{61b}$$

From the Ewald-Oseen extinction theorem for the electric field (Eq. (25)) it follows that the sum of the right hand sides of Eqs. (53a) and (61a) is equal to zero.

Similarly, from the Ewald-Oseen extinction theorem for the magnetic field (Eq. (27)), it follows that the sum of the right hand sides of Eqs. (53b) and (61b) is equal to zero. Since this is valid for all points in the lattice, i.e., for all (p,q), we conclude that $\boldsymbol{\beta}=\mathbf{k}_\rho$. We define the unknown state vectors $B^{(M)}(\mathbf{K})$, $B^{(E)}(\mathbf{K})$ with components $B^{(M)}_{lm}(\mathbf{K}), B^{(E)}_{lm}(\mathbf{K})$, respectively. We define the matrices $\Omega^{(1)}(\mathbf{k}_\rho)$, $\Omega^{(2)}(\mathbf{k}_\rho)$ with components $\Omega^{(1)}_{lm;l'm'}(\mathbf{k}_\rho), \Omega^{(2)}_{lm;l'm'}(\mathbf{k}_\rho)$ and the vectors $A^{(MS)}(\mathbf{K})$, $A^{(ES)}(\mathbf{K})$ with components $A^{(MS)}_{lm}(\mathbf{K}), A^{(ES)}_{lm}(\mathbf{K})$, respectively. Notice that $B^{(M)}_{lm}, B^{(E)}_{lm}$ are related to $A^{(M)}_{lm}, A^{(E)}_{lm}$ by means of Eqs. (46a) and (46b). Finally, we define the diagonal matrices

$$T^{(M)}_{lm;l'm'} = \frac{\beta^{(M)}_l}{\alpha^{(M)}_l} \delta_{ll'}\delta_{mm'}, \tag{62a}$$

$$T^{(E)}_{lm;l'm'} = \frac{\beta^{(E)}_l}{\alpha^{(E)}_l} \delta_{ll'}\delta_{mm'}. \tag{62b}$$

Then, for each wavevector $\mathbf{K}$ of the source field, the state vectors $B^{(M)}(\mathbf{K})$, $B^{(E)}(\mathbf{K})$ are computed from the following linear algebraic system:

$$\left[I - T^{(M)}\Omega^{(1)}(\mathbf{k}_\rho)\right]B^{(M)}(\mathbf{K}) - T^{(M)}\Omega^{(2)}(\mathbf{k}_\rho)B^{(E)}(\mathbf{K}) = T^{(M)}A^{(MS)}(\mathbf{K}), \tag{63a}$$

$$-T^{(E)}\Omega^{(2)}(\mathbf{k}_\rho)B^{(M)}(\mathbf{K}) + \left[I - T^{(E)}\Omega^{(1)}(\mathbf{k}_\rho)\right]B^{(E)}(\mathbf{K}) = T^{(E)}A^{(ES)}(\mathbf{K}), \tag{63b}$$

where I is the identity matrix. The series in Eqs. (54a), (54b), are independent of the origin $\mathbf{a}_{pq}$ in $\hat{\mathbf{a}}_{p'q'} = \mathbf{a}_{p'q'} - \mathbf{a}_{pq}$, and, therefore, we have the relations:

$$\Omega^{(1)}_{lm;l'm'}(\mathbf{k}_\rho) = \frac{1}{\zeta_l} \sum_{p'q'}{}' e^{-j\mathbf{k}_\rho \cdot \mathbf{a}_{p'q'}} U_{l'm';lm}(\mathbf{a}_{p'q'}) \tag{64a}$$

$$\Omega^{(2)}_{lm;l'm'}(\mathbf{k}_\rho) = \frac{1}{\zeta_l} \sum_{p'q'}{}' e^{-j\mathbf{k}_\rho \cdot \mathbf{a}_{p'q'}} U_{l'm';lm}(\mathbf{a}_{p'q'}). \tag{64b}$$

The linear algebraic system above is almost the same to that in the paper by A. Modinos [5]. He is using Bessel and Hankel functions, while we are using modified Bessel functions. The main difference is in the functions $U_{lm;l'm'}(\mathbf{r}_0)$, $V_{lm;l'm'}(\mathbf{r}_0)$, (Eqs. (55a), (55b)), which in our

case are expressed in integral form. This will allow us to transform $\Omega^{(1)}(\mathbf{k}_\rho)$, $\Omega^{(2)}(\mathbf{k}_\rho)$ from the real domain into the spectral domain. But the uniqueness of the solution of Maxwell's equations ensures that, in real space, the solution to the linear algebraic system above gives the same fields to those of A. Modinos' paper.

Next, we consider the scattered fields outside the spheres, i.e., when $|\mathbf{r}-\mathbf{a}_{pq}|>R$ for all (p,q). In this case, for each wavevector $\mathbf{K}$ of the source field, the scattered electric field is equal to

$$E^{(sc)}_{2,\mathbf{K}}(\mathbf{r}) = \sum_{pq} e^{-j\mathbf{k}_\rho \cdot \mathbf{a}_{pq}} j \sum_{lm} \left[B^{(M)}_{lm}(\mathbf{K}) \mathbf{E}^{(M,out)}_{2,lm}(\mathbf{r}_{pq}) + B^{(E)}_{lm}(\mathbf{K}) \mathbf{E}^{(E,out)}_{2,lm}(\mathbf{r}_{pq}) \right]. \tag{65}$$

If we use the identity (III 23) in Appendix III, where we set $\sigma = \sigma_2$, we obtain the relation

$$\begin{aligned} \mathbf{E}^{(sc)}_{2,\mathbf{K}}(\mathbf{r}) &= \frac{j}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\lambda_x d\lambda_y}{\sigma_2 \tilde{\gamma}_2} e^{-j\lambda\cdot\rho - \tilde{\gamma}_2 |z|} \\ &* \sum_{lm} \left[B^{(M)}_{lm}(\mathbf{K}) \tilde{\mathbf{Y}}^{M}_{ll_l} \left((\mathrm{sign} z) \frac{\tilde{\gamma}_2}{\sigma_2}, \varphi_\lambda \right) \right. \\ &\left. + B^{(E)}_{lm}(\mathbf{K}) \frac{1}{j\sigma_2} (-j\lambda - (\mathrm{sign} z) \tilde{\gamma}_2 \mathbf{e}_z) \times \tilde{\mathbf{Y}}^{m}_{lll} \left((\mathrm{sign} z) \frac{\tilde{\gamma}_2}{\sigma_2}, \varphi_\lambda \right) \right] \\ &* \sum_{pq} e^{-j(\mathbf{k}_\rho - \lambda)\cdot \mathbf{a}_{pq}}, \end{aligned} \tag{66}$$

where

$$\tilde{\gamma}_2 = \left[\lambda^2 + \sigma_2^2 \right]^{1/2}. \tag{67}$$

Here, $\tilde{\mathbf{Y}}^{M}_{lll}(w, \varphi_\lambda)$ are the complex vector spherical harmonics, where $Y_{l'm-\mu}(\Omega_r)$ is replaced by $Y_{l'm-\mu}(w, \varphi_\lambda)$ in Eq. (I2a) in appendix I. Also, the scattered field is computed outside the spheres. Therefore, we must have $|z| \geq R$.

Eq. (66) can be rewritten in the spectral domain by using the transition relation

$$\sum_{pq} e^{-j(\mathbf{k}_\rho - \lambda)\cdot \mathbf{a}_{pq}} \rightarrow \frac{(2\pi)^2}{S_c} \sum_{p',q'} \delta^{(2)}(\lambda - \mathbf{k}_\rho - \mathbf{b}_{p'q'}), \tag{68}$$

where S_c is the area of the unit cell in real space and $\mathbf{b}_{pq}$ has already been defined (Eqs. (48a), (48b), (49)). The scattered electric field becomes equal to

$$\mathbf{E}_{2,\mathbf{K}}^{(sc)}(\mathbf{r}) = j\frac{2\pi}{S_c}\sum_{\mathbf{K}'}\frac{1}{\sigma_2\gamma_2'}e^{-j\mathbf{K}'\cdot\boldsymbol{\rho}-\gamma_2|z|}\sum_{lm}\Bigg[B_{lm}^{(M)}(\mathbf{K})\widetilde{\mathbf{Y}}_{lll}^{M}((\text{signz})\frac{\gamma_2'}{\sigma_2},\varphi_{\mathbf{K}'}) + B_{lm}^{(E)}(\mathbf{K})\frac{1}{j\sigma_2}(-j\mathbf{K}'-(\text{signz})\gamma_2'\mathbf{e}_z)\times\widetilde{\mathbf{Y}}_{lll}^{m}((\text{signz})\frac{\gamma_2'}{\sigma_2},\varphi_{\mathbf{K}'})\Bigg], \tag{69}$$

where

$$\gamma_2' = \left[\mathbf{K}'^2 + \sigma_2^2\right]^{1/2}. \tag{70}$$

We have omitted the subscripts p',q' in $\mathbf{K}_{p'q'} \equiv \mathbf{k}_\rho + \mathbf{b}_{p'q'}$ to simplify the notation. A straightforward computation leads to the following two relations

$$[l(l+1)]^{1/2}\widetilde{\mathbf{Y}}_{lll}^{m}((\text{signz})\frac{\gamma_2}{\sigma_2},\varphi_{\mathbf{K}}) = (\text{signz})^{l-m+1}\left[C_{lm}^{(TM)}\hat{\mathbf{K}} + C_{lm}^{(TE)}(e_z\times\hat{\mathbf{K}})\right] + (\text{signz})^{l-m}D_{lm}^{(TM)}\mathbf{e}_z, \tag{71a}$$

$$\left(-jK\hat{\mathbf{K}}-(\text{signz})\gamma_2\mathbf{e}_z\right)\times[l(l+1)]^{1/2}\widetilde{\mathbf{Y}}_{lll}^{m}\left((\text{signz})\frac{\gamma_2}{\sigma_2},\varphi_{\mathbf{K}}\right) = (\text{signz})^{l-m}\left[\gamma_2 C_{lm}^{(TE)}\hat{\mathbf{K}} - \frac{\sigma_2^2}{\gamma_2}C_{lm}^{(TM)}\left(\mathbf{e}_z\times\hat{\mathbf{K}}\right)\right] - (\text{signz})^{l-m+1}jKC_{lm}^{(TE)}\mathbf{e}_z, \tag{71b}$$

where

$$C_{lm}^{(TM)} = \alpha_l^m\widetilde{Y}_{l,m+1}\left(\frac{\gamma_2}{\sigma_2},\varphi_{\mathbf{K}}\right)e^{-j\varphi_{\mathbf{K}}} + \beta_l^m\widetilde{Y}_{l,m-1}\left(\frac{\gamma_2}{\sigma_2},\varphi_{\mathbf{K}}\right)e^{j\varphi_{\mathbf{K}}}, \tag{72a}$$

$$C_{lm}^{(TE)} = -j\left[\alpha_l^m\widetilde{Y}_{l,m+1}\left(\frac{\gamma_2}{\sigma_2},\varphi_{\mathbf{K}}\right)e^{-j\varphi_{\mathbf{K}}} - \beta_l^m\widetilde{Y}_{l,m-1}\left(\frac{\gamma_2}{\sigma_2},\varphi_{\mathbf{K}}\right)e^{j\varphi_{\mathbf{K}}}\right], \tag{72b}$$

$$D_{lm}^{(TM)} = m\widetilde{Y}_{lm}\left(\frac{\gamma_2}{\sigma_2},\varphi_{\mathbf{K}}\right) = -\frac{jK}{\gamma_2}C_{lm}^{(TM)}. \tag{72c}$$

Here, $\hat{\mathbf{K}}$ is the unit vector and K the magnitude of $\mathbf{K}$. Substitution of Eqs. (71a), (71b) into the scattered electric field, yields the following relation in the plane wave representation, when $|z|>R$:

$$\mathbf{E}_{2,\mathbf{K}}^{(sc)}(\mathbf{r}) = \sum_{\mathbf{K}'} e^{-j\mathbf{K}'\cdot\rho}\left\{\Theta(z-R)e^{-\gamma_2'(z-R)}\left[E_{\mathbf{K}',sc}^{(TE+)}(R)\left(\mathbf{e}_z \times \hat{\mathbf{K}}'\right) + E_{\mathbf{K}',sc}^{(TM+)}(R)\left(\hat{\mathbf{K}}' - \frac{jK'}{\gamma_2'}\mathbf{e}_z\right)\right]\right. , \quad (73)$$

$$\left. + \Theta(-z-R)e^{\gamma_2'(z+R)}\left[E_{\mathbf{K}',sc}^{(TE-)}(-R)\left(\mathbf{e}_z \times \hat{\mathbf{K}}'\right) + E_{\mathbf{K}',sc}^{(TM-)}(-R)\left(\hat{\mathbf{K}}' + \frac{jK'}{\gamma_2'}\mathbf{e}_z\right)\right]\right\}$$

where

$$E_{\mathbf{K}',sc}^{(TE+)}(R) = \frac{2\pi}{S_c}e^{-\gamma_2' R}\sum_{lm}\frac{1}{[l(l+1)]^{1/2}}\left[\frac{1}{\sigma_2\gamma_2'}C_{lm}^{(TE)}B_{lm}^{(M)}(\mathbf{K}) - \frac{1}{\gamma_2'^2}C_{lm}^{(TM)}(\mathbf{K})B_{lm}^{(E)}(\mathbf{K})\right] \quad (74a)$$

$$E_{\mathbf{K}',sc}^{(TM+)}(R) = \frac{2\pi}{S_c}e^{-\gamma_2' R}\sum_{lm}\frac{1}{[l(l+1)]^{1/2}} * \left[\frac{j}{\omega_2\gamma_2'}C_{lm}^{(TM)}B_{lm}^{(M)}(\mathbf{K}) + \frac{1}{\sigma_2^2}C_{lm}^{(TE)}B_{lm}^{(E)}(\mathbf{K})\right], \quad (74b)$$

$$E_{\mathbf{K}',sc}^{(TE-)}(-R) = \frac{2\pi}{S_c}e^{-\gamma_2' R}\sum_{lm}\frac{(-1)^{l-m+1}}{[l(l+1)]^{1/2}} * \left[\frac{j}{\sigma_2\gamma_2'}C_{lm}^{(TE)}B_{lm}^{(M)}(\mathbf{K}) + \frac{1}{\gamma_2'^2}C_{lm}^{(TM)}B_{lm}^{(E)}(\mathbf{K})\right], \quad (74c)$$

$$E_{\mathbf{K}',sc}^{(TM-)}(-R) = \frac{2\pi}{S_c}e^{-\gamma_2' R}\sum_{lm}\frac{(-1)^{l-m+1}}{[l(l+1)]^{1/2}} * \left[\frac{j}{\sigma_2\gamma_2'}C_{lm}^{(TM)}B_{lm}^{(M)}(\mathbf{K}) - \frac{1}{\sigma_2^2}C_{lm}^{(TE)}B_{lm}^{(E)}(\mathbf{K})\right]. \quad (74d)$$

The scattered magnetic field is computed from the curl of the electric field and is equal to

$$\mathbf{H}_{2,\mathbf{K}}^{(sc)}(\mathbf{r}) = \frac{\sigma_2}{j\omega\mu_0}\sum_{\mathbf{K}'} e^{-j\mathbf{K}'\cdot\rho}\left\{\Theta(z-R)e^{-\gamma_2'(z-R)}\left[\frac{\sigma_2}{\gamma_2'}E_{\mathbf{K}',sc}^{(TM+)}(R)(\mathbf{e}_z \times \hat{\mathbf{K}}')\right.\right.$$

$$\left. - E_{\mathbf{K}',sc}^{(TE+)}(R)\left(\frac{\gamma_2'}{\sigma_2}\hat{\mathbf{K}}' - \frac{jK'}{\sigma_2}\mathbf{e}_z\right)\right] + \Theta(-z-R)e^{\gamma_2'(z+R)}\left[-\frac{\sigma_2}{\gamma_2'}E_{\mathbf{K}',sc}^{(TM-)}(-R)(\mathbf{e}_z \times \hat{\mathbf{K}}'),\right. \quad (75)$$

$$\left.\left. + E_{\mathbf{K}',sc}^{(TE-)}(-R)\left(\frac{\gamma_2'}{\sigma_2}\hat{\mathbf{K}}' + \frac{jK'}{\sigma_2}\mathbf{e}_z\right)\right]\right\}$$

At this point, we introduce the scattering matrix that relates the fields at z=-R and z=R by means of the relation

$$\begin{bmatrix} E_{\mathbf{K}',sc}^{(TE-)}(-R) \\ E_{\mathbf{K}',sc}^{(TM-)}(-R) \\ E_{\mathbf{K}',sc}^{(TE+)}(R) \\ E_{\mathbf{K}',sc}^{(TM+)}(R) \end{bmatrix} = S_{\mathbf{K}'\mathbf{K}} \begin{bmatrix} E_{\mathbf{K}}^{(TE+)}(-R) \\ E_{\mathbf{K}}^{(TM+)}(-R) \\ E_{\mathbf{K}}^{(TE-)}(R) \\ E_{\mathbf{K}}^{(TM-)}(R) \end{bmatrix}. \quad (76)$$

The components of the right-hand vector are the amplitudes of the source electric field (of Eq. (57a)) while the components of the left-hand vector are the amplitudes of the scattered electric field (cf. Eqs. (73), (74a)-(74d)). The matrix elements of $S_{\mathbf{K}'\mathbf{K}}$ are obtained by solving the algebraic system in Eqs. (63a), (63b) for each of the four individual cases where one of the components of the right-hand vector in Eq. (76) is set equal to one, and the rest are zero. Then, in each case, we use the solutions for $B^{(M)}(\mathbf{K}), B^{(E)}(\mathbf{K})$ to compute the scattered amplitudes from Eqs. (74a)-(74d) and identify them as the elements of $S_{\mathbf{K}'\mathbf{K}}$.

If we divide $S_{\mathbf{K}'\mathbf{K}}$ into submatrices, i.e.,

$$S_{\mathbf{K}'\mathbf{K}} = \begin{bmatrix} S^{(1,1)}_{\mathbf{K}'\mathbf{K}} & S^{(1,2)}_{\mathbf{K}'\mathbf{K}} \\ S^{(2,1)}_{\mathbf{K}'\mathbf{K}} & S^{(2,2)}_{\mathbf{K}'\mathbf{K}} \end{bmatrix}, \tag{77}$$

then $S^{(1,1)}_{\mathbf{K}'\mathbf{K}}, S^{(1,2)}_{\mathbf{K}'\mathbf{K}}$ give the (TE) and (TM) reflected and transmitted amplitudes of the electric field at z=–R and z=+R, respectively, with wavevector $\mathbf{K}'$, if the source field is either a forward (TE) or (TM) wave at z=–R with wavevector $\mathbf{K}$. Similarly, $S^{(2,2)}_{\mathbf{K}'\mathbf{K}}, S^{(1,2)}_{\mathbf{K}'\mathbf{K}}$ give the reflected and transmitted amplitudes at z=+R and z=–R, respectively, if the source field is a backward wave at z=+R. We see then that the scattering matrix $S_{\mathbf{K}'\mathbf{K}}$ contains all the information about the scattering of a plane wave by the array of dielectric spheres.

The total field at z=–R and z=R is the sum of the source field and the scattered field. If we define, for the total field, the two-component vectors

$$E^{(+)}_{\mathbf{K}}(R) = \begin{bmatrix} E^{(TE+)}_{\mathbf{K}}(R) \\ E^{(TM+)}_{\mathbf{K}}(R) \end{bmatrix}, \tag{78a}$$

$$E^{(-)}_{\mathbf{K}}(R) = \begin{bmatrix} E^{(TE-)}_{\mathbf{K}}(R) \\ E^{(TM-)}_{\mathbf{K}}(R) \end{bmatrix}, \tag{78b}$$

and similar vectors $E^{(+)}_{\mathbf{K}}(-R), E^{(-)}_{\mathbf{K}}(-R)$ at z=–R, then it follows from Eqs. (57a), (76), (77) that

$$E^{(-)}_{\mathbf{K}'}(-R) = S^{(1,1)}_{\mathbf{K}'\mathbf{K}} E^{(+)}_{\mathbf{K}}(-R) + \left(e^{-2\gamma_2 R}\delta_{\mathbf{K}'\mathbf{K}} I_{2\times 2} + S^{(1,2)}_{\mathbf{K}'\mathbf{K}}\right) E^{(-)}_{\mathbf{K}}(R). \tag{79a}$$

$$E^{(+)}_{\mathbf{K}'}(R) = \left(e^{-2\gamma_2 R}\delta_{\mathbf{K}'\mathbf{K}} I_{2\times 2} + S^{(2,1)}_{\mathbf{K}'\mathbf{K}}\right) E^{(+)}_{\mathbf{K}}(-R) + S^{(2,2)}_{\mathbf{K}'\mathbf{K}} E^{(-)}_{\mathbf{K}}(R), \tag{79b}$$

where $I_{2\times 2}$ is the 2×2 identity matrix and $\delta_{\mathbf{K}'\mathbf{K}} = 1$ if $\mathbf{K}' = \mathbf{K}$ and zero otherwise. Here, we added the amplitudes of the source field to the transmitted components of the scattered field. In matrix form, Eqs. (79a), (79b) can be written as follows:

$$\begin{bmatrix} E_{\mathbf{K}'}^{(-)}(-R) \\ E_{\mathbf{K}'}^{(+)}(R) \end{bmatrix} = \begin{bmatrix} \tilde{S}_{\mathbf{K}'\mathbf{K}}^{(1,1)}(-R,R) & \tilde{S}_{\mathbf{K}'\mathbf{K}}^{(1,2)}(-R,R) \\ \tilde{S}_{\mathbf{K}'\mathbf{K}}^{(2,1)}(-R,R) & \tilde{S}_{\mathbf{K}'\mathbf{K}}^{(2,2)}(-R,R) \end{bmatrix} \begin{bmatrix} E_{\mathbf{K}}^{(+)}(-R) \\ E_{\mathbf{K}}^{(-)}(R) \end{bmatrix}, \tag{80a}$$

where

$$\tilde{S}_{\mathbf{K}'\mathbf{K}}^{(1,1)}(-R,R) = S_{\mathbf{K}'\mathbf{K}}^{(1,1)}, \tag{80b}$$

$$\tilde{S}_{\mathbf{K}'\mathbf{K}}^{(1,2)}(-R,R) = e^{-2\gamma_2 R}\delta_{\mathbf{K}'\mathbf{K}} I_{2\times 2} + S_{\mathbf{K}'\mathbf{K}}^{(1,2)}, \tag{80c}$$

$$\tilde{S}_{\mathbf{K}'\mathbf{K}}^{(2,1)}(-R,R) = e^{-2\gamma_2 R}\delta_{\mathbf{K}'\mathbf{K}} I_{2\times 2} + S_{\mathbf{K}'\mathbf{K}}^{(2,1)}, \tag{80d}$$

$$\tilde{S}_{\mathbf{K}'\mathbf{K}}^{(2,2)}(-R,R) = S_{\mathbf{K}'\mathbf{K}}^{(2,2)}. \tag{80d}$$

In the relation above, both the right-hand and left-hand vectors refer to the amplitude of the total electric field at z=–R and z=R.

Given the total scattering matrix $\tilde{S}_{\mathbf{K}'\mathbf{K}}(-R,R)$, it is easy to obtain the total scattering matrix $\tilde{S}_{\mathbf{K}'\mathbf{K}}(-z_1,z_2)$ that refers to the amplitudes at $z=-z_1$ and $z=z_2$, where $z_1 \geq R$, $z_2 \geq R$, using the propagation matrices. From Eqs. (57a), (73), we see that

$$E_{\mathbf{K}}^{(+)}(z_2) = P_{\mathbf{K}}(z_2 \leftarrow -z_1) E_{\mathbf{K}}^{(+)}(-z_1), \tag{81a}$$

$$E_{\mathbf{K}}^{(-)}(z_2) = P_{\mathbf{K}}^{-1}(z_2 \leftarrow -z_1) E_{\mathbf{K}}^{(-)}(-z_1), \tag{81b}$$

where

$$P_{\mathbf{K}}(z_2 \leftarrow -z_1) = e^{-\gamma_2 (z_2 + z_1)} I_{2\times 2}, \tag{82a}$$

$$P_{\mathbf{K}}^{-1}(z_2 \leftarrow -z_1) = e^{\gamma_2 (z_2 + z_1)} I_{2\times 2}. \tag{82b}$$

Substitution of Eqs. (81a), (81b) into Eq. (80a) leads to the relation

$$\begin{bmatrix} E_{\mathbf{K}'}^{(-)}(-z_1) \\ E_{\mathbf{K}'}^{(+)}(z_2) \end{bmatrix} = \tilde{S}_{\mathbf{K}'\mathbf{K}}(-z_1,z_2) \begin{bmatrix} E_{\mathbf{K}}^{(+)}(-z_1) \\ E_{\mathbf{K}}^{(-)}(z_2) \end{bmatrix}, \tag{83a}$$

where

$$\tilde{S}_{\mathbf{K}'\mathbf{K}}(-z_1,z_2) = \begin{bmatrix} \tilde{S}_{\mathbf{K}'\mathbf{K}}^{(1,1)}(-z_1,z_2) & \tilde{S}_{\mathbf{K}'\mathbf{K}}^{(1,2)}(-z_1,z_2) \\ \tilde{S}_{\mathbf{K}'\mathbf{K}}^{(2,1)}(-z_1,z_2) & \tilde{S}_{\mathbf{K}'\mathbf{K}}^{(2,2)}(-z_1,z_2) \end{bmatrix}, \tag{83b}$$

and

$$\widetilde{S}^{(1,1)}_{\mathbf{K'K}}(-z_1,z_2) = e^{-(\gamma'_2+\gamma_2)(z_1-R)}\widetilde{S}^{(1,1)}_{\mathbf{K'K}}(-R,R)\,, \tag{84a}$$

$$\widetilde{S}^{(1,2)}_{\mathbf{K'K}}(-z_1,z_2) = e^{-\gamma'_2(z_1-R)-\gamma_2(z_2-R)}\widetilde{S}^{(1,2)}_{\mathbf{K'K}}(-R,R)\,, \tag{84b}$$

$$\widetilde{S}^{(2,1)}_{\mathbf{K'K}}(-z_1,z_2) = e^{-\gamma'_2(z_2-R)-\gamma_2(z_1-R)}\widetilde{S}^{(2,1)}_{\mathbf{K'K}}(-R,R)\,, \tag{84c}$$

$$\widetilde{S}^{(2,2)}_{\mathbf{K'K}}(-z_1,z_2) = e^{-(\gamma'_2+\gamma_2)(z_2-R)}\widetilde{S}^{(2,2)}_{\mathbf{K'K}}(-R,R)\,. \tag{84d}$$

The transfer matrix $T(z_2 \leftarrow -z_1)$ can be easily obtained from Eqs. (83a), (83b) by constructing the state vector that refers to all the wavevectors **K** under consideration. We group together all the backward waves and all the forward waves and define the four state vectors

$$E_2^{(\alpha)}(\tilde{z}) = \begin{bmatrix} E^{(\alpha)}_{\mathbf{K}_1}(\tilde{z}) \\ E^{(\alpha)}_{\mathbf{K}_2}(\tilde{z}) \\ \vdots \\ E^{(\alpha)}_{\mathbf{K}_N}(\tilde{z}) \end{bmatrix}, \tag{85}$$

where $\alpha = (+)$ or $(-)$, i.e., forward or backward wave (of Eq. (78a), (78b)) and $\tilde{z} = -z_1$ or z_2. Then, it follows from Eqs. (83a), (83b) that

$$E_2^{(-)}(-z_1) = \widetilde{S}^{(1,1)}E_2^{(+)}(-z_1) + \widetilde{S}^{(1,2)}E_2^{(-)}(z_2)\,, \tag{86a}$$

$$E_2^{(+)}(z_2) = \widetilde{S}^{(2,1)}E_2^{(+)}(-z_1) + \widetilde{S}^{(2,2)}E_2^{(-)}(z_2)\,, \tag{86b}$$

where the matrix elements of $\widetilde{S}^{(i,j)}$ are equal to $\widetilde{S}^{(i,j)}_{m,n} = \widetilde{S}^{(i,j)}_{\mathbf{K}_m\mathbf{K}_n}(-z_1,z_2)$, m=1,2,…,N, n=1,2,…,N. The transfer matrix is computed from the algebraic system of Eqs. (86a), (86b), and expressed by the relation

$$\begin{bmatrix} E_2^{(+)}(z_2) \\ E_2^{(-)}(z_2) \end{bmatrix} = \widetilde{T}(z_2 \leftarrow -z_1)\begin{bmatrix} E_2^{(+)}(-z_1) \\ E_2^{(-)}(-z_1) \end{bmatrix}, \tag{87a}$$

where

$$\widetilde{T}(z_2 \leftarrow -z_1) = \begin{bmatrix} \widetilde{S}^{(2,1)} - \widetilde{S}^{(2,2)}\widetilde{S}^{(1,2)^{-1}}\widetilde{S}^{(1,1)} & \widetilde{S}^{(2,2)}\widetilde{S}^{(1,2)^{-1}} \\ -\widetilde{S}^{(1,2)^{-1}}\widetilde{S}^{(1,1)} & \widetilde{S}^{(1,2)^{-1}} \end{bmatrix}. \tag{87b}$$

The computation of the transfer matrix allows us to superimpose many layers of dielectric spheres at the same or different distances between them and compute the transfer matrix, as well as, the scattering matrix of the total set of layers.

The wavevectors $\mathbf{K}_{pq}$ that should be included in the state vectors above (cf. Eq. (85)) are for all the propagating modes. In a non-absorptive host medium, where the real part of σ_2 tends to zero, a pair of integers (p,q) for which $\gamma_2(\mathbf{K}_{pq})$ (cf. Eqs. (58), (70)) is purely imaginary (in the limit where $\mathrm{Re}(\sigma_2) \to 0$), defines a propagating mode in medium 2 (cf. Eqs. (84a)-(84d)). In particular, the mode for the source field for which p=q=0, is the principal propagating mode. The rest of the modes are evanescent. In addition to the fact that the amplitudes associated with them decay exponentially with distance (cf. Eqs. (84a)-(84d)), their radiated power is equal to zero, i.e., they do not contribute to the reflection and transmission coefficients. Therefore, there is no need for them to be included in the state vectors. On the other hand, in an absorptive host medium where σ_2, has a positive real part, we define the propagating modes as the pairs (p,q) for which $\gamma_2(\mathbf{K}_{pq})$ satisfies the criterion $|\mathrm{Im}(\gamma_2)/\gamma_2| > \varepsilon$. Here, ε is a small positive number, e.g., $\varepsilon = 0.001$, that should be adjusted so that the rest of the modes have a negligible contribution in the radiated power by the array of dielectric spheres.

IV. $\Omega^{(1)}_{lm;l'm'}(\mathbf{r}_0), \Omega^{(2)}_{lm;l'm'}(\mathbf{r}_0)$ in the real and spectral domain

The functions $\Omega^{(1)}_{lm;l'm'}(\mathbf{r}_0), \Omega^{(2)}_{lm;l'm'}(\mathbf{r}_0)$ are given by Eqs. (64a), (64b) and the functions $U_{lm;l'm'}(\mathbf{r}_0), V_{lm;l'm'}(\mathbf{r}_0)$ are given by Eqs. (55a), (55b). In Appendices IV and V the scalar and vector addition theorems are derived. Thus, from the vector addition theorem, i.e, Eq. (V1), we obtain the relation

$$\mathbf{E}^{(M,out)}_{2,lm}(\mathbf{r}-\mathbf{r}_0) = \sum_{l'm'} \left[\widetilde{U}_{lm;l'm'}(\mathbf{r}_0)\mathbf{E}^{(M,in)}_{2,l'm'}(\mathbf{r}) + \widetilde{V}_{lm;l'm'}(\mathbf{r}_0)\mathbf{E}^{(E,in)}_{2,l'm'}(\mathbf{r}) \right], \tag{88}$$

where $\widetilde{U}_{lm;l'm'}(\mathbf{r}_0), \widetilde{V}_{lm;l'm'}(\mathbf{r}_0)$ are given by Eqs. (V2a), (V2b), and $\sigma = \sigma_2$ in these equations. Similarly, from Eq. (V3), are obtained the relation

$$\mathbf{E}^{(E,out)}_{2,lm}(\mathbf{r}-\mathbf{r}_0) = \sum_{lm} \left[\widetilde{U}_{lm;l'm'}(\mathbf{r}_0)\mathbf{E}^{(M,in)}_{2,lm}(\mathbf{r}) + \widetilde{V}_{lm;l'm'}(\mathbf{r}_0)\mathbf{E}^{(E,in)}_{2,lm}(\mathbf{r}) \right]. \tag{89}$$

Substitution of Eq. (88) into Eq. (55a) and Eq. (89) into Eq. (55b), together with the orthonormality of the vector spherical harmonics and the definition of ζ_l (cf. Eq. (56)) lead to the relations

$$U_{lm;l'm'}(\mathbf{r}_0) = \zeta_l \widetilde{U}_{lm;l'm'}(\mathbf{r}_0), \tag{90a}$$

$$V_{lm;l'm'}(\mathbf{r}_0) = \zeta_l \widetilde{V}_{lm;l'm'}(\mathbf{r}_0). \tag{90b}$$

Therefore, in the real domain, $\Omega^{(1)}_{lm;l'm'}(\mathbf{r}_0), \Omega^{(2)}_{lm;l'm'}(\mathbf{r}_0)$ (cf. Eqs. (64a), (64b)) are given by the following relations:

$$\begin{aligned}\Omega^{(1)}_{l'm';lm}(\mathbf{k}_\rho) &= \frac{1}{[l(l+1)l'(l'+1)]^{1/2}} \\ &* \left[2\alpha^m_l \beta^{m'+1}_{l'} \widetilde{Z}^{l',m'+1}_{l,m+1}(\mathbf{k}_\rho) + 2\alpha^{m'-1}_{l'} \beta^m_l \widetilde{Z}^{l',m'-1}_{l,m-1}(\mathbf{k}_\rho) + mm'\widetilde{Z}^{l'm'}_{lm}(\mathbf{k}_\rho) \right]'\end{aligned} \tag{91a}$$

$$\Omega^{(2)}_{l'm';lm}(\mathbf{k}_\rho) = \frac{2l'+1}{[l(l+1)l'(l'+1)]^{1/2}}(-1)^{m'}\sqrt{\frac{4\pi}{3}}$$
$$* \Big[\sqrt{2}\alpha_l^m B_{l'-1,m'+1}(1,-1;l'm')\widetilde{Z}^{l'-1,m'+1}_{l,m+1}(\mathbf{k}_\rho) \qquad (91b)$$
$$-\sqrt{2}\beta_l^m B_{l'-1,m'-1}(1,1;l'm')\widetilde{Z}^{l'-1,m'-1}_{l,m-1}(\mathbf{k}_\rho)$$
$$+ mB_{l'-1,m'}(1,0;l'm')\widetilde{Z}^{l'-1,m'}_{l,m}(\mathbf{k}_\rho)\Big],$$

where

$$\widetilde{Z}^{l'm'}_{lm}(\mathbf{k}_\rho) = \sum_{pq}{}' e^{-j\mathbf{k}_\rho\cdot\mathbf{a}_{pq}}\widetilde{G}_{lm;l'm'}(\mathbf{a}_{pq}), \qquad (92)$$

and $\widetilde{G}_{lm;l'm'}(\mathbf{a}_{pq})$ is given by Eq. (IV 2), where $\sigma = \sigma_2$.

These expressions are identical to those in the paper by A. Madinos [5] except for the function $\widetilde{G}_{lm;l'm'}(\mathbf{a}_{pq})$ since he is using Hankel functions while we are using modified Bessel functions. We see then that the integral equation approach provides the same solution as the approach of applying the boundary conditions at the surface of the dielectric spheres.

The computation of $\Omega^{(1)}_{lm;l'm'}(\mathbf{k}_\rho), \Omega^{(2)}_{lm;l'm'}(\mathbf{k}_\rho)$ in the spectral domain requires the Fourier transforms of the vector functions in Eqs. (55a), (55b), which are derived in Appendix VI. In terms of the Fourier transforms, i.e., Eqs. (VI 8a) – (VI 8c), Eqs. (55a), (55b) become equal to

$$U_{lm;l'm'}(\mathbf{r}_0) = \frac{1}{(2\pi)^3}\int \hat{\mathbf{E}}^{(M,out)}_{2,lm}(\lambda)\cdot\hat{\mathbf{E}}^{(M,in)^*}_{2,lm}(\lambda)e^{j\lambda\cdot\mathbf{r}_0}d^3\lambda, \qquad (93a)$$

$$V_{lm;l'm'}(\mathbf{r}_0) = \frac{1}{(2\pi)^3}\int \hat{\mathbf{E}}^{(E,out)}_{2,lm}(\lambda)\cdot\hat{\mathbf{E}}^{(M,in)^*}_{2,lm}(\lambda)e^{j\lambda\cdot\mathbf{r}_0}d^3\lambda, \qquad (93b)$$

the integration extending over the whole space in the spectral domain. Notice that, when $\mathbf{r}_0 = \mathbf{0}$ in Eqs. (55a), (55b) then the functions $E^{(\alpha,out)}_{2,lm}(\mathbf{r})$, where $\alpha = M, E$, are zero inside V_0 and the functions $U_{lm,l'm'}(\mathbf{0}), V_{lm;l'm'}(\mathbf{0})$ are zero. Therefore, when the integral form of U and V is used, then the prime in Eqs. (64a), (64b) can be removed, i.e., the term with p=q=0 can be included in the summation. Thus, substitution of Eqs. (93a), (93b) into Eqs. (64a), (64b) and application of the transition relation in Eq. (68), leads to the relations

$$\Omega^{(1)}_{l'm';lm}(\mathbf{k}_\rho) = \frac{1}{\zeta_l}\frac{1}{S_c}\sum_{\mathbf{K}}\frac{1}{2\pi}\int_{-\infty}^{\infty}\hat{\mathbf{E}}^{(M,in)^*}_{2,l'm'}(\mathbf{K},\lambda_z)\cdot\hat{\mathbf{E}}^{(M,out)}_{2,lm}(\mathbf{K},\lambda_z)d\lambda_z \qquad (94a)$$

$$\Omega^{(2)}_{l'm';lm}(\mathbf{k}_\rho) = \frac{1}{\zeta_{l'}}\frac{1}{S_c}\sum_{\mathbf{K}}\frac{1}{2\pi}\int_{-\infty}^{\infty}\hat{\mathbf{E}}^{(M,in)^*}_{2,l'm'}(\mathbf{K},\lambda_z)\cdot\mathbf{E}^{(E,out)}_{2,lm}(\mathbf{K},\lambda_z)d\lambda_z \qquad (94b)$$

where $\mathbf{K}_{pq} = \mathbf{k}_\rho + \mathbf{b}_{pq}$, and the summation is over all (p,q) points in the reciprocal lattice. The subscripts (p,q) have been omitted in Eqs. (94a), (94b) for simplicity of notation.

Next, we compute the right hand side of Eq. (94a). From the definition of the vector spherical harmonics (cf. Eqs. (I1a), (V9)), we obtain the relation

$$\begin{aligned}
&\mathbf{Y}_{l'l'1}^{m'^*}(\Omega_\lambda)\cdot\mathbf{Y}_{ll1}^{m}(\Omega_\lambda)=\frac{1}{[l(l+1)l'(l'+1)]^{1/2}}\\
&*\Big[2\alpha_{l'}^{m'}\alpha_l^m Y_{l',m'+1}^*(\Omega_\lambda)Y_{l,m+1}(\Omega_\lambda)+2\beta_{l'}^{m'}\beta_l^m Y_{l',m'-1}^*(\Omega_\lambda)Y_{l,m-1}(\Omega_\lambda),\\
&+mm'Y_{l'm'}^*(\Omega_\lambda)Y_{lm}(\Omega_\lambda)\Big]
\end{aligned}\tag{95}$$

where $\lambda=(\lambda_\rho,\lambda_z)$ and $\lambda_\rho=\mathbf{K}_{pq}$. Substitution of Eqs. (IV 8a), (VI 8b), (95) into Eq. (94a) leads to the relation

$$\begin{aligned}
&\Omega_{l'm';lm}^{(1)}(\mathbf{k}_\rho)=\frac{1}{[l(l+1)l'(l'+1)]^{1/2}}\\
&*\Big[2\alpha_l^m\beta_{l'}^{m'+1}Z_{l,m+1}^{l',m'+1}(\mathbf{k}_\rho)+2\alpha_{l'}^{m'-1}\beta_l^m Z_{l,m-1}^{l',m'-1}(\mathbf{k}_\rho)+mm'Z_{lm}^{l'm'}(\mathbf{k}_\rho)\Big],
\end{aligned}\tag{96}$$

where

$$Z_{lm}^{l'm'}(\mathbf{k}_\rho)=\frac{8\pi R^2}{S_c\zeta_{l'}}\sum_{\mathbf{K}}\int_{-\infty}^{\infty}\frac{F_{l'}^*(\lambda,\sigma_2)}{\lambda_z^2+\gamma_2^{*2}}\,\frac{G_l(\lambda,\sigma_2)}{\lambda_z^2+\gamma_2^2}\,Y_{l'm'}^*(\Omega_\lambda)Y_{lm}(\Omega_\lambda)d\lambda_z\tag{97}$$

$$\gamma_2^2=\mathbf{K}^2+\sigma_2^2\tag{98}$$

The functions $F_l(\lambda,\sigma_2), G_l(\lambda,\sigma_2)$ are given by Eqs. (VI 3b), (VI 4b), respectively. Also, $\lambda=\left(\lambda_\rho^2+\lambda_z^2\right)^{1/2}$, where $\lambda_\rho=\mathbf{K}_{pq}$ and $\mathbf{K}_{pq}=\mathbf{k}_\rho+\mathbf{b}_{pq}, \mathbf{b}_{pq}$ being a vector in the reciprocal lattice. Notice that Eqs. (91a), (96) are identical except for $\tilde{Z}_{lm}^{l'm'}(\mathbf{k}_\rho)$ being replaced by $Z_{lm}^{l'm'}(\mathbf{k}_\rho)$. It is rather obvious then that we should have the identity

$$\tilde{Z}_{lm}^{l'm'}(\mathbf{k}_\rho)=Z_{lm}^{l'm'}(\mathbf{k}_\rho).\tag{99}$$

In Appendix VII it is shown that this is the case. Eqs. (96), (97) provide $\Omega_{l'm';lm}^{(1)}(\mathbf{k}_\rho)$ in the spectral domain and Eq. (91b) provides $\Omega_{l'm';lm}^{(2)}(\mathbf{k}_\rho)$ in the spectral domain if $\tilde{Z}_{lm}^{l'm'}(\mathbf{k}_\rho)$ is replaced by $Z_{lm}^{l'm'}(\mathbf{k}_\rho)$.

The integral in Eq. (97) can be computed analytically only when **K=0**, i.e., for normal incidence of the source wave and at the origin of the reciprocal lattice. In the general case, the integral can be expressed as a series of terms involving modified Bessel functions. The explicit expression of the series will be given elsewhere. Therefore, the computation of $Z_{lm}^{l'm'}(\mathbf{k}_\rho)$ in Eq. (97) involves a three-dimensional summation, as compared to a two-dimensional summation for the computation of $\tilde{Z}_{lm}^{l'm'}(\mathbf{k}_\rho)$ in Eq. (92). On the other hand, for large values of (p,q), the sum in Eq. (97) is of order $\left|\mathbf{K}_{pq}\right|^{-3}$ (after the integral has been expressed as a series), while the

sum in Eq. (92) is of order $\left|\mathbf{a}_{pq}\right|^{-1}$. Therefore, in a lossless medium, the sum in $Z_{lm}^{l'm'}(\mathbf{k}_\rho)$ should converge much faster than that in $\tilde{Z}_{lm}^{l'm'}(\mathbf{k}_\rho)$, notwithstanding the third sum due to the integral in Eq. (97). Due to the oscillatory behavior of the terms in Eq. (92), the maximum values of (p,q) must be at least equal to 10^4 in order to obtain the plot in Fig. 3 in the paper by N. Stefanou [6]. Therefore, $4*10^8$ terms are required in the sum of Eq. (92) for convergence. On the other hand, some preliminary results using Eq. (97) indicate that the maximum values of (p,q) must be equal to 50 and the number of terms in the sum for the integral should be 200. Therefore, there are $5*10^5$ terms to be summed in Eq. (97). Thus, there is an advantage to perform the computations in the spectral domain rather than in the real domain for lossless host medium. On the other hand, in a lossy host medium, for sufficiently high absorption $\tilde{Z}_{lm}^{l'm'}(\mathbf{k}_\rho)$ will converge faster than $Z_{lm}^{l'm'}(\mathbf{k}_\rho)$ due to the exponentially decaying terms in the modified Bessel functions (cf. Eqs. (92), (IV9), (I7b)).

V. Multilayer and Three-Dimensional Array of Spheres

When there are more than one layer of dielectric spheres, each layer is obtained from the previous one by shifting all the spheres of the latter layer by the vector $\mathbf{a}_3$. At the zeroth layer, which lies at z=0, if the spheres are located at $\mathbf{a}_{pq}$, then at the n^{th} layer the spheres are located at $\mathbf{a}_{pq} + n\mathbf{a}_3$. The translation of the spheres from $\mathbf{a}_{pq}$, at z=0 to $\mathbf{a}_{pq}+n\mathbf{a}_{pq}$ is equivalent to moving the coordinates of the n^{th} layer from $\mathbf{r}$ to $\mathbf{r}$-$n\mathbf{a}_3$. Therefore, for the n^{th} layer, instead of Eq. (73), the scattering amplitudes at $z=\pm\frac{1}{2}a_{3z}$, where z is measured from the n^{th} layer, become:

$$E_{\mathbf{K}',sc}^{(+)}(n;\tfrac{1}{2}a_{3z}) = e^{j\mathbf{K}'\cdot n\mathbf{a}_3 - \gamma_2'(\frac{1}{2}a_{3z}-R)} E_{\mathbf{K}',sc}^{(+)}(R), \tag{100a}$$

$$E_{\mathbf{K}',sc}^{(-)}(n;-\tfrac{1}{2}a_{3z}) = e^{j\mathbf{K}'\cdot n\mathbf{a}_3 - \gamma_2'(\frac{1}{2}a_{3z}-R)} E_{\mathbf{K}',sc}^{(-)}(-R). \tag{100b}$$

Also, for the n^{th} layer, instead of Eq. (57a), the amplitudes for the sourse field at $z=\pm\frac{1}{2}a_{3z}$ are:

$$E_{\mathbf{K}}^{(+)}(n;-\tfrac{1}{2}a_{3z}) = e^{j\mathbf{K}\cdot n\mathbf{a}_3 + \gamma_2\left(\frac{1}{2}a_{3z}-R\right)} E_{\mathbf{K}}^{(+)}(-R), \tag{101a}$$

$$E_{\mathbf{K}}^{(-)}(n;\tfrac{1}{2}a_{3z}) = e^{j\mathbf{K}\cdot n\mathbf{a}_3 + \gamma_2\left(\frac{1}{2}a_{3z}-R\right)} E_{\mathbf{K}}^{(-)}(R). \tag{101b}$$

On the left hand side of the relations above, the first index indicates the layer and the second index is the value of z (measured from the n^{th} layer) where the amplitudes are computed. By adding the amplitudes of the source field to the transmitted components of the scattered field from $z=-\frac{1}{2}a_{3z}$ to $z=\frac{1}{2}a_{3z}$, instead of Eqs. (80a)-(80d) we obtain the following relation for the scattering matrix of the n^{th} layer:

$$\begin{bmatrix} E_{\mathbf{K}'}^{(-)}(n;-\tfrac{1}{2}a_{3z}) \\ E_{\mathbf{K}'}^{(+)}(n;\tfrac{1}{2}a_{3z}) \end{bmatrix} = e^{j(\mathbf{K}'-\mathbf{K})\cdot n\mathbf{a}_3} * \begin{bmatrix} \widetilde{S}_{\mathbf{K}'\mathbf{K}}^{(1,1)}(-\tfrac{1}{2}a_{3z},\tfrac{1}{2}a_{3z}) & \widetilde{S}_{\mathbf{K}'\mathbf{K}}^{(1,2)}(-\tfrac{1}{2}a_{3z},\tfrac{1}{2}a_{3z}) \\ \widetilde{S}_{\mathbf{K}'\mathbf{K}}^{(2,1)}(-\tfrac{1}{2}a_{3z},\tfrac{1}{2}a_{3z}) & \widetilde{S}_{\mathbf{K}'\mathbf{K}}^{(2,2)}(-\tfrac{1}{2}a_{3z},\tfrac{1}{2}a_{3z}) \end{bmatrix} \begin{bmatrix} E_{\mathbf{K}}^{(+)}(n;-\tfrac{1}{2}a_{3z}) \\ E_{\mathbf{K}}^{(-)}(n;\tfrac{1}{2}a_{3z}) \end{bmatrix} \tag{102}$$

where $\widetilde{S}_{\mathbf{K}'\mathbf{K}}^{(i,j)}(-z_1,z_2)$ is given by Eqs. (84a)-(84d). If we define vectors similar to those of Eq. (85) for the n^{th} layer and also define the diagonal matrix

$$G(\mathbf{A}) = \begin{bmatrix} e^{-jK_1\cdot\mathbf{A}} & & 0 \\ & e^{-jK_2\cdot\mathbf{A}} & \\ 0 & & \ddots e^{-jK_N\cdot\mathbf{A}} \end{bmatrix}, \tag{103}$$

then, instead of Eqs. (86a), (86b), we obtain the relation

$$\begin{bmatrix} G(n\mathbf{a}_3)E^{(-)}(n;-\tfrac{1}{2}a_{3z}) \\ G(n\mathbf{a}_3)E^{(+)}(n;\tfrac{1}{2}a_{3z}) \end{bmatrix} = \begin{bmatrix} \widetilde{S}^{(1,1)} & \widetilde{S}^{(1,2)} \\ \widetilde{S}^{(2,1)} & \widetilde{S}^{(2,2)} \end{bmatrix} \begin{bmatrix} G(n\mathbf{a}_3)E^{(+)}(n;-\tfrac{1}{2}a_{3z}) \\ G(n\mathbf{a}_3)E^{(-)}(n;\tfrac{1}{2}a_{3z}) \end{bmatrix}. \tag{104}$$

The transfer matrix is computed from the relation above for the n^{th} layer, from the plane at $z = -\frac{1}{2}a_{3z}$ to the plane at $z = \frac{1}{2}a_{3z}$, namely,

$$E(n+1) = \widetilde{G}(-n\mathbf{a}_3)\widetilde{T}(\tfrac{1}{2}a_{3z} \leftarrow -\tfrac{1}{2}a_{3z})\widetilde{G}(n\mathbf{a}_3)E(n), \tag{105}$$

where

$$E(n) = \begin{bmatrix} E^{(+)}(n;-\tfrac{1}{2}a_{3z}) \\ E^{(-)}(n;-\tfrac{1}{2}a_{3z}) \end{bmatrix}, \tag{106a}$$

$$E(n+1) = \begin{bmatrix} E^{(+)}(n;\tfrac{1}{2}a_{3z}) \\ E^{(-)}(n;\tfrac{1}{2}a_{3z}) \end{bmatrix}, \tag{106b}$$

$$\widetilde{G}(\mathbf{A}) = \begin{bmatrix} G(\mathbf{A}) & 0 \\ 0 & G(\mathbf{A}) \end{bmatrix}, \tag{107}$$

and $\widetilde{T}(z_2 \leftarrow -z_1)$ is given by Eq. (87b).

For n layers, it follows from Eq. (105) that

$$E(n) = \widetilde{G}(-(n-\tfrac{1}{2})\mathbf{a}_3)\hat{T}^n\widetilde{G}(-\tfrac{1}{2}\mathbf{a}_3)E(0), \tag{108}$$

where

$$\hat{T} = \widetilde{G}(\tfrac{1}{2}\mathbf{a}_3)\widetilde{T}(\tfrac{1}{2}a_{3z} \leftarrow -\tfrac{1}{2}a_{3z})\widetilde{G}(\tfrac{1}{2}a_3). \tag{109}$$

Eq. (108) can also be written as follows:

$$\hat{E}(n) = \hat{T}^n \hat{E}(0), \tag{110}$$

where

$$\hat{E}(n) = \widetilde{G}((n - \tfrac{1}{2})\mathbf{a}_3)E(n). \tag{111}$$

Then, for two consecutive layers we have the relation

$$\hat{E}(n+1) = \hat{T}\hat{E}(n). \tag{112}$$

For a three-dimensional lattice, i.e., when there is an infinite number of layers, application of the Bloch theorem, namely,

$$E(n+1) = e^{jk_z a_{3z}} E(n), \tag{113}$$

leads to the homogeneous algebraic system

$$\left[\hat{T} - e^{jk_z a_{3z}} I\right]\hat{E}(n) = 0. \tag{114}$$

The dispersion relation of the three-dimensional lattice, i.e., k_z as a function of (k_x,k_y,ω) is determined by the determinant in Eq. (114) being set equal to zero. Following this procedure, we can compute the propagating modes, as well as the band gaps in the infinite lattice.

Another approach to determine the disperson relation of the infinite lattice is as follows: Let the unit cell of the three dimensional lattice be determined by the translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, so that the lattice points are given by $\mathbf{a}_{pqr}=p\mathbf{a}_1+q\mathbf{a}_z+r\mathbf{a}_3$. The fundamental vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ of the reciprocal lattice are given by the usual expressions in term of $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ and they satisfy the relations $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$. Notice that, if $\mathbf{a}_3 \cdot \mathbf{e}_z \neq 0$, then $\mathbf{b}_1$, $\mathbf{b}_2$ are not parallel to $\mathbf{B}_1$, $\mathbf{B}_2$ in Eqs. (48a), (48b). The points in the reciprocal lattice are given by $\widetilde{\mathbf{b}}_{pqr} = p\mathbf{b}_1 + q\mathbf{b}_2 + r\mathbf{b}_3$. Following the same steps in Section III, we conclude that $\Omega^{(1)}, \Omega^{(2)}$ in Eqs. (64a), (64b) become functions of the three-dimensional vector $\mathbf{k}$, the sums are over (p,q,r) and $\mathbf{k}_\rho$, $\mathbf{a}_{pq}$ are replaced by $\mathbf{k}$, $\mathbf{a}_{pqr}$, respectively. The dispersion relation of the lattice is determined by setting the right-hand side in Eqs. (63a), (63b) equal to zero, and computing the values of $k_z=f(k_x, k_y, \omega)$ for which the determinant of the left-hand side is equal to zero. The functions $\Omega^{(1)}(\mathbf{k})$, $\Omega^{(2)}(\mathbf{k})$ are still given by Eqs. (91a), (91b), (92), where the sums are over (p,q,r) and $\mathbf{k}_\rho$, $\mathbf{a}_{pq}$ are replaced by $\mathbf{k}$, $\mathbf{a}_{pqr}$, respectively. Thus, Eq. (92) becomes

$$\widetilde{Z}_{lm}^{l'm'}(\mathbf{k}) = \sum_{pqr} e^{-j\mathbf{k}\cdot\mathbf{a}_{pqr}} \widetilde{G}_{lm;l'm'}(\mathbf{a}_{pqr}), \tag{115}$$

where $\widetilde{G}_{lm;l'm'}(\mathbf{a}_{pqr})$ is given by Eq. (IV 2) and $\sigma = \sigma_2$. Also, Eq. (99) is still valid, except that, in the three-dimensional case, Eq. (97) becomes equal to

$$Z_{lm}^{l'm'}(\mathbf{k}) = \frac{16\pi^2 R}{V_c \zeta_{l'}} \sum_{pqr} \frac{F_{l'}^*\left(\left|\mathbf{K}_{pqr}\right|, \sigma_2\right)}{\mathbf{K}_{pqr}^2 + \sigma_2^{*2}} \frac{G_l\left(\left|\mathbf{K}_{pqr}\right|, \sigma_2\right)}{\mathbf{K}_{pqr}^2 + \sigma_2^2} Y_{l'm'}^*\left(\Omega_{\mathbf{K}_{pqr}}\right) Y\left(\Omega_{\mathbf{K}_{pqr}}\right) \tag{116}$$

Here, V_c is the volume of the unit cell and $\mathbf{K}_{pqr} = \mathbf{k} + \widetilde{\mathbf{b}}_{pqr}$. In a lossless host medium, we see that $\widetilde{Z}_{lm}^{l'm'}(\mathbf{k})$ is of order $\left|\mathbf{a}_{pqr}\right|^{-1}$, while $Z_{lm}^{l'm'}(\mathbf{k})$ is of order $\left|\mathbf{K}_{pqr}\right|^{-4}$. Therefore, the sum in Eq. (116) converges much faster than that in Eq. (115). On the other hand, in a lossy host medium, for sufficiently high absorption, $\widetilde{Z}_{lm}^{l'm'}(\mathbf{k})$ converges faster than $Z_{lm}^{l'm'}(\mathbf{k})$ due to the exponentially decaying terms in the modified Bessel functions (cf. Eqs. (115), (IV 9), (I 7b)). It is only through actual computation that can be determined whether Eq. (115) or Eq. (116) should be used in the presence of a lossy host medium.

VI. The Array of Spheres Embedded in a Slab

The slab is medium 2 with complex wave number σ_2 (cf. Eq. (1)) and lies between the planes at $z=-z_1$ and $z=z_2$ (z_1, z_2 are positive). The medium 1 for $z>z_2$ has wavenumber σ_1 and the medium 4 for $z<-z_1$ has wavenumber σ_4. Here, we consider the general case, while, in most cases, media 1 and 4 are the vacuum. The two-dimensional array of spheres lies at z=0, and its scattering matrix is given by Eqs. (86a), (86b), namely,

$$\begin{bmatrix} E_2^{(-)}(-z_1) \\ E_2^{(+)}(z_2) \end{bmatrix} = \widetilde{S} \begin{bmatrix} E_2^{(+)}(-z_1) \\ E_2^{(-)}(z_2) \end{bmatrix}. \tag{117}$$

For a multilayer array, the scattering matrix can be obtained from Eq. (108) and, therefore, Eq. (117) covers this case too.

The vectors $E_2^{(\pm)}(-z_1), E_2^{(\pm)}(z_2)$ are given by Eq. (85), i.e., they refer to all the wavevectors $\mathbf{K}$ relevant to the computation (cf. the paragraph at the end of Section III).

Application of the boundary conditions for the electromagnetic field at $z=-z_1$, $z=z_2$ for each wavevector $\mathbf{K}$ yields the relations

$$t_{24} E_2^{(+)}(-z_1) = E_4^{(+)}(-z_1) + r_{24} E_4^{(-)}(-z_1), \tag{118a}$$

$$t_{24} E_2^{(-)}(-z_1) = r_{24} E_4^{(+)}(-z_1) + E_4^{(-)}(-z_1), \tag{118b}$$

$$t_{12} E_1^{(+)}(z_2) = E_2^{(+)}(z_2) + r_{12} E_2^{(-)}(z_2), \tag{118c}$$

$$t_{12} E_1^{(-)}(z_2) = r_{12} E_2^{(+)}(z_2) + E_2^{(-)}(z_2). \tag{118d}$$

Here, r_{ij}, t_{ij} are diagonal 2Nx2N matrices with diagonal elements $r_{ij}^{(TE)}(\mathbf{K}_1)$, $r_{ij}^{(TM)}(\mathbf{K}_1)$, ..., $r_{ij}^{(TE)}(\mathbf{K}_N)$, $r_{ij}^{(TM)}(\mathbf{K}_N)$ and $t_{ij}^{(TE)}(\mathbf{K}_1)$, $t_{ij}^{(TM)}(\mathbf{K}_1)$, ..., $t_{ij}^{(TE)}(\mathbf{K}_N)$, $t_{ij}^{(TM)}(\mathbf{K}_N)$, respectively, where

$$r_{ij}^{(TE)}(\mathbf{K}) = \frac{\gamma_i - \gamma_j}{\gamma_i + \gamma_j}, \tag{119a}$$

$$t_{ij}^{(TE)}(\mathbf{K}) = \frac{2\gamma_i}{\gamma_i + \gamma_j}, \tag{119b}$$

$$r_{ij}^{(TM)}(\mathbf{K}) = \frac{\sigma_i^2 \gamma_j - \sigma_j^2 \gamma_i}{\sigma_i^2 \gamma_j + \sigma_j^2 \gamma_i}, \tag{119c}$$

$$t_{ij}^{(TM)}(\mathbf{K}) = \frac{2\sigma_i^2\gamma_j}{\sigma_i^2\gamma_j+\sigma_j^2\gamma_i}, \tag{119d}$$

$$\gamma_l = \left[\mathbf{K}^2 + \sigma_l^2\right]^{1/2}. \tag{119e}$$

Also, the subscript i in $E_i^{(\pm)}(z)$, denotes the medium where the amplitudes are computed.

Rearranging Eqs. (118a) – (118d), we obtain the following relations

$$\begin{bmatrix} E_2^{(+)}(-z_1) \\ E_2^{(-)}(z_2) \end{bmatrix} = A\begin{bmatrix} E_4^{(+)}(-z_1) \\ E_1^{(-)}(z_2) \end{bmatrix} - B\begin{bmatrix} E_2^{(-)}(-z_1) \\ E_2^{(+)}(z_2) \end{bmatrix}, \tag{120a}$$

$$\begin{bmatrix} E_4^{(-)}(-z_1) \\ E_1^{(+)}(z_2) \end{bmatrix} = B\begin{bmatrix} E_4^{(+)}(-z_1) \\ E_1^{(-)}(z_2) \end{bmatrix} + D\begin{bmatrix} E_2^{(-)}(-z_1) \\ E_2^{(+)}(z_2) \end{bmatrix}, \tag{120b}$$

where

$$A = \begin{bmatrix} I - r_{24} & 0 \\ 0 & t_{12} \end{bmatrix}, \tag{121a}$$

$$B = \begin{bmatrix} -r_{24} & 0 \\ 0 & r_{12} \end{bmatrix}, \tag{121b}$$

$$D = \begin{bmatrix} t_{24} & 0 \\ 0 & I - r_{12} \end{bmatrix}. \tag{121c}$$

Here I,0 are the 2Nx2N unit and zero matrices, respectively. The solution of the algebraic system of Eqs. (117), (120a), (120b) yields the relation

$$\begin{bmatrix} E_4^{(-)}(-z_1) \\ E_1^{(+)}(z_2) \end{bmatrix} = \hat{S}\begin{bmatrix} E_4^{(+)}(-z_1) \\ E_1^{(-)}(z_2) \end{bmatrix}, \tag{122}$$

where

$$\hat{S} = B + D\tilde{S}\left[I + B\tilde{S}\right]^{-1}A. \tag{123}$$

$\hat{S}$ is the total scattering matrix for the total amplitudes computed just outside the slab and, therefore, it provides the reflection and transmission coefficients of the array outside the slab.

VII. Reflection and Transmission Coefficients

From the previous section we see that, if the source and scattered field have wavevectors $\mathbf{k}_\rho$ and $\mathbf{K}'$, respectively, then their amplitudes in media 1 and 4 are related by the elements of the total scattering matrix in Eq. (122), namely,

$$\begin{bmatrix} E_{4\mathbf{K}'}^{(TE-)}(-z_1) \\ E_{4\mathbf{K}'}^{(TM-)}(-z_1) \\ E_{1\mathbf{K}'}^{(TE+)}(z_2) \\ E_{1\mathbf{K}'}^{(TM+)}(z_2) \end{bmatrix} = \hat{S}(\mathbf{K}',\mathbf{k}_\rho) \begin{bmatrix} E_{4\mathbf{k}_\rho}^{(TE+)}(-z_1) \\ E_{4\mathbf{k}_\rho}^{(TM+)}(-z_1) \\ E_{1\mathbf{k}_\rho}^{(TE-)}(z_2) \\ E_{1\mathbf{k}_\rho}^{(TM-)}(z_2) \end{bmatrix}. \tag{124}$$

The power flux in medium i, at z and through the area S_c of the unit cell is equal to

$$P_i(z) = \mathrm{Re} \int_{S_c}\!\!\int \left[\mathbf{E}_i^*(\rho,z) \times \mathbf{H}_i(\rho,z)\right] \cdot \mathbf{e}_z dxdy. \tag{125}$$

In the plane wave representation (cf. Eqs. (57a), (57b), (73), (75)), the power flux for the forward (+) and backward (−) waves becomes equal to

$$P_i^{(\pm)}(z) = S_c \sum_{\mathbf{K}'} \left[\mathrm{Re}\left(\frac{\gamma_i(\mathbf{K}')}{j\omega\mu_0}\right) \left|E_{i,\mathbf{K}'}^{(TE\pm)}(z)\right|^2 + \mathrm{Re}\left(\frac{\sigma_i^2}{j\omega\mu_0\gamma_i(\mathbf{K}')}\right) \left|E_{i,\mathbf{K}'}^{(TM\pm)}(z)\right|^2 \right], \tag{126}$$

where

$$\gamma_i(\mathbf{K}') = \left[\mathbf{K}'^2 + \sigma_i^2\right]^{1/2}. \tag{127}$$

Thus, for a backward source field in medium 1, the power flux for the (TE−) and (TM−) source waves at $z=z_2$, are equal to

$$P_{1,\mathbf{k}_\rho}^{(TE-)}(z_2) = S_c \,\mathrm{Re}\left(\frac{\gamma_1(\mathbf{k}_\rho)}{j\omega\mu_0}\right) \left|E_{1,\mathbf{k}_\rho}^{(TE-)}(z_2)\right|^2, \tag{128a}$$

$$P_{1,\mathbf{k}_\rho}^{(TM-)}(z_2) = S_c \,\mathrm{Re}\left(\frac{\sigma_1^2}{j\omega\mu_0\gamma_1(\mathbf{k}_\rho)}\right) \left|E_{1,\mathbf{k}_\rho}^{(TM-)}(z_2)\right|^2. \tag{128b}$$

Similar expressions are obtained for the source field in medium 4.

The reflection and transmission coefficients follow from Eqs. (124), (126), (128a), (128b). For example, if the source field is a (TE−) wave with wavevector $\mathbf{k}_\rho$ in medium 1, then the total reflection coefficient at $z=z_2$ is equal to

$$\mathcal{R}_1(\mathbf{k}_\rho, TE) = 1 - \frac{1}{\mathrm{Re}(-j\gamma_1)} * \sum_{\mathbf{K}'} \left[\mathrm{Re}\left[(-j\gamma_1')\left(\delta_{\mathbf{K}',\mathbf{k}\rho} - \hat{S}_{33}(\mathbf{K}',\mathbf{k}_\rho)\right)\left(\delta_{\mathbf{K}',\mathbf{k}\rho} + \hat{S}_{33}^*(\mathbf{K}',\mathbf{k}_\rho)\right)\right] + \mathrm{Re}\left(\frac{\sigma_1^2}{j\gamma_1'}\right)\left|\hat{S}_{43}(\mathbf{K}',\mathbf{k}_\rho)\right|^2 \right] \tag{129}$$

where $\gamma_1 = \left[\mathbf{k}_\rho^2 + \sigma_1^2\right]^{1/2}, \gamma_1' = \left[\mathbf{K}'^2 + \sigma_1^2\right]^{1/2}$. The total transmission coefficient at $z=-z_1$ is equal to

$$\mathcal{T}_4(\mathbf{k}_\rho, TE) = \frac{1}{\mathrm{Re}(-j\gamma_1)} \sum_{\mathbf{K}'} \left[\mathrm{Re}(-j\gamma_4')\left|\hat{S}_{13}(\mathbf{K}',\mathbf{k}_\rho)\right|^2 + \mathrm{Re}\left(\frac{\sigma_4^2}{j\gamma_4'}\right)\left|\hat{S}_{23}(\mathbf{K}',\mathbf{k}_\rho)\right|^2 \right] \tag{130}$$

On the other hand, if the source field is a (TM–) wave in medium 1, then the total reflection coefficient at $z=z_2$ is equal to

$$\mathcal{R}_1(\mathbf{k}_\rho,\mathrm{TM}) = 1 - \frac{1}{\mathrm{Re}\left(\frac{\sigma_1^2}{j\gamma_1}\right)} * \sum_{\mathbf{K}'}\left[\mathrm{Re}(-j\gamma_1')\left|\hat{S}_{34}(\mathbf{K}',\mathbf{k}_\rho)\right|^2 + \mathrm{Re}\left[\frac{\sigma_1^2}{j\gamma_1'}\left(\delta_{\mathbf{K}',\mathbf{k}\rho} - \hat{S}_{44}(\mathbf{K}',\mathbf{k}_\rho)\right)\left(\delta_{\mathbf{K}',\mathbf{k}\rho} + \hat{S}_{44}^*(\mathbf{K}',\mathbf{k}_\rho)\right)\right]\right] \tag{131}$$

and the total transmission coefficient at $z=-z_1$ is equal to

$$\mathcal{J}_4(\mathbf{k}_\rho,\mathrm{TM}) = \frac{1}{\mathrm{Re}\left(\frac{\sigma_1^2}{j\gamma_1}\right)}\sum_{\mathbf{K}'}\left[\mathrm{Re}(-j\gamma_4')\left|\hat{S}_{14}(\mathbf{K}',\mathbf{k}_\rho)\right|^2 + \mathrm{Re}\left(\frac{\sigma_4^2}{j\gamma_4'}\right)\left|\hat{S}_{24}(\mathbf{K}',\mathbf{k}_\rho)\right|^2\right] \tag{132}$$

where $\gamma_4' = \left[\mathbf{K}'^2 + \sigma_4^2\right]^{1/2}$. Similar expressions can be obtained if the source field is a forward (+) field in medium 4. Notice, that each individual term in the sums in Eqs. (129)-(132) provides information as to how much each individual wavevector $\mathbf{K}$ contributes to the total reflection and transmission coefficients. In the case when the host medium or the spheres between the planes at $z=-z_1$ and $z=z_2$ are lossy, the absorption coefficient $\mathcal{A}$, is equal to

$$\mathcal{A} = 1 - \mathcal{R} - \mathcal{J}, \tag{133}$$

where $\mathcal{R}$, $\mathcal{J}$ refer to each case mentioned above for the reflection and transmission coefficients.

VIII. Summary and Conclusions

A semi-analytic integral equation approach was presented in this paper for the computation of the reflection and transmission coefficients by a single or multi-layer array of dielectric spheres embedded in a host medium. It was shown that this approach is equivalent to that of applying the boundary conditions at the surface of the spheres. The integral equation formalism is simple in its application only for special shapes of scattering objects such as non-overlapping spheres or cylinders of infinite extent in the z-direction with circular or rectangular cross section, embedded in a host medium. In these cases there is a complete set of functions to expand the electric and magnetic currents. No restriction is imposted on the lattice two- or three-dimensional configuration.

Both the homogeneous (eigenvalue) and inhomogeneous (plane wave source) problem were formulated. Two approaches were presented for the three-dimensional eigenvalue problem, either by the application of the Bloch theorem (cf. Eqs. (113), (114)) or by solving the homogeneous algebraic system in Eqs. (63a), (63b) where the right hand side is set equal to zero.

The integral equation approach provides an easy transition from the real to the spectral domain either in the two- or three-dimentional lattice of dielectric spheres. In Appendix VII, the proof that the identity in Eq. (99) is valid, is rather simple. But it was only after the integral equation approach was applied that it became evident that $\widetilde{Z}_{lm}^{l'm'}$ as given by Eqs. (92), (115) in the real domain is identical to $Z_{lm}^{l'm'}$ as given by Eqs. (97), (116) in the spectral domain.

In a lossless host medium, the sums in $Z_{lm}^{l'm'}$ should converge much faster in the spectral domain rather, than in the real domain. Therefore, the computation of the scattered fields and the reflection and transmission coefficients should be faster. In addition, as it was shown in the paper by N. Stefanou, et. al. [6] (cf. Table 1 in their paper), a small value of l_{max} (where $l=1,2,\ldots,l_{max}$) is sufficient for an accurate computation of the scattered fields. Consequently, the size of the matrices involved in the computation is small. Therefore, there is a small requirement for memory as well as computer time. Furthermore, due to the small size of the matrices, the poor convergence problems for hard spheres in the plane-wave method or the unstable solutions in the transfer matrix method, should not arise here. In conclusion, the approach presented here, although limited, could be used as a benchmark to compare and check the results by more advanced and elaborate approaches such as the plane wave expansion or the transfer matrix approach.

Appendix I

Most of the following relations are taken from reference [19]. The vector spherical harmonics are defined as follows:

$$\mathbf{Y}^m_{lll}(\Omega_r) = -\frac{j}{[l(l+1)]^{1/2}}(\mathbf{r}\times\nabla)Y_{lm}(\Omega_r), \tag{I1a}$$

$$\mathbf{Y}^m_{l,l+1,l}(\Omega_r) = \frac{r^{l+2}}{[(l+1)(2l+1)]^{1/2}}\nabla(r^{-l-1}Y_{lm}(\Omega_r)), \tag{I1b}$$

$$\mathbf{Y}^m_{l,l-1,l}(\Omega_r) = \frac{r^{-l+1}}{[l(2l+1)]^{1/2}}\nabla(r^{l}Y_{lm}(\Omega_r)), \tag{I1c}$$

where $\Omega_r \equiv (\theta,\varphi)$, l=1,2,3,…, m=-l,-l+1,…,l-1,l, and $Y_{lm}(\Omega_r)$ are the scalar spherical harmonics. For computational purposes, the vector spherical harmonics can be expressed in terms of the 3j-symbol [19] as follows:

$$\mathbf{Y}^m_{ll'1}(\Omega_r) = \sum_{\mu=-1}^{1}(2l+1)^{1/2}(-1)^{l-m}\begin{pmatrix} l & l' & 1 \\ m & -m+\mu & -\mu \end{pmatrix} Y_{l',m-\mu}(\Omega_r)\mathbf{e}_\mu\,, \tag{I2a}$$

where $l' = l-1, l, l+1$, and

$$\mathbf{e}_{\pm1} = \mp\frac{1}{\sqrt{2}}(\mathbf{e}_x \pm \mathbf{e}_y), \tag{I2b}$$

$$\mathbf{e}_0 = \mathbf{e}_z \tag{I2c}$$

Here, $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ are the unit vectors along the three axes in cartesian coordinates.

The vector spherical harmonics form an orthonormal set, i.e.,

$$\int \mathbf{Y}^{m'*}_{ll'1}(\Omega_r)\cdot\mathbf{Y}^{m''}_{l''l''1}(\Omega_r)d\Omega_r = \delta_{ll''}\delta_{l'l''}\delta_{m'm''}. \tag{I3}$$

The integration is over the 4π-solid angle. Moreover, they satisfy the identities

$$\mathbf{e}_r\cdot\mathbf{Y}^m_{lll}(\Omega_r) = 0, \tag{I4a}$$

$$\mathbf{e}_r\cdot\mathbf{Y}^m_{l,l+1,l}(\Omega_r) = -\left(\tfrac{l+1}{2l+1}\right)^{1/2}Y_{lm}(\Omega_r), \tag{I4b}$$

$$\mathbf{e}_r\cdot\mathbf{Y}^m_{l,l-1,l}(\Omega_r) = \left(\tfrac{l}{2l+1}\right)^{1/2}Y_{lm}(\Omega_r), \tag{I4c}$$

and

$$\mathbf{e}_r\times\mathbf{Y}^m_{lll}(\Omega_r) = j\left[\left(\tfrac{l}{2l+1}\right)^{1/2}\mathbf{Y}_{l,l+1,l}(\Omega_r) + \left(\tfrac{l+1}{2l+1}\right)^{1/2}\mathbf{Y}^m_{l,l-1,l}(\Omega_r)\right], \tag{I5a}$$

$$\mathbf{e}_r\times\mathbf{Y}^m_{l,l+1,l}(\Omega_r) = j\left(\tfrac{l}{2l+1}\right)^{1/2}\mathbf{Y}^m_{lll}(\Omega_r), \tag{I5b}$$

$$\mathbf{e}_r\times\mathbf{Y}^m_{l,l-1,l}(\Omega_r) = j\left(\tfrac{l+1}{2l+1}\right)^{1/2}\mathbf{Y}^m_{lll}(\Omega_r). \tag{I5c}$$

With the help of Eqs. (I1a)-(I1c) and (I5a)-(I5c) it can be shown that:

$$\nabla \times \mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}) = j\left(\tfrac{l}{2l+1}\right)^{1/2}\left(-\tfrac{l}{r}\right)\mathbf{Y}_{l,l+1,1}^{m}(\Omega_{\mathbf{r}}) + j\left(\tfrac{l+1}{2l+1}\right)^{1/2}\tfrac{l+1}{r}\mathbf{Y}_{l,l-1,1}^{m}(\Omega_{\mathbf{r}}), \tag{I6a}$$

$$\nabla \times \mathbf{Y}_{l,l+1,1}^{m}(\Omega_{\mathbf{r}}) = j\left(\tfrac{l}{2l+1}\right)^{1/2}\tfrac{l+2}{r}\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}), \tag{I6b}$$

$$\nabla \times \mathbf{Y}_{l,l-1,1}^{m}(\Omega_{\mathbf{r}}) = -j\left(\tfrac{l+1}{2l+1}\right)^{1/2}\tfrac{l-1}{r}\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}). \tag{I6c}$$

The modified spherical Bessel functions of the first and third kind [20] are defined as follows:

$$f_l(z) = \left(\frac{\pi/2}{z}\right)^{1/2} I_{l+1/2}(z), \tag{I7a}$$

$$g_l(z) = \left(\frac{1}{\frac{\pi}{2}z}\right) K_{l+1/2}(z), \tag{I7b}$$

where z can be a complex number. Notice that $g_l(z)$ here defers by a factor $\pi/2$ to that defined in Abramowitz. They satisfy the identities:

$$\left(\tfrac{d}{dz} - \tfrac{l}{z}\right) f_l(z) = f_{l+1}(z), \tag{I8a}$$

$$\left(\tfrac{d}{dz} + \tfrac{l+1}{z}\right) f_l(z) = f_{l-1}(z), \tag{I8b}$$

$$\left(\tfrac{d}{dz} - \tfrac{l}{z}\right) g_l(z) = -g_{l+1}(z), \tag{I8c}$$

$$\left(\tfrac{d}{dz} + \tfrac{l+1}{z}\right) g_l(z) = -g_{l-1}(z). \tag{I8d}$$

From these identities and Eqs. (I6a)-(I6c), the following relations can be shown to be valid:

$$\nabla \times f_l(\sigma r)\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}) = j\sigma\left[\left(\tfrac{l}{2l+1}\right)^{1/2} f_{l+1}(\sigma r)\mathbf{Y}_{l,l+1,1}^{m}(\Omega_{\mathbf{r}}) + \left(\tfrac{l+1}{2l+1}\right)^{1/2} f_{l-1}(\sigma r)\mathbf{Y}_{l,l-1,1}^{m}(\Omega_{\mathbf{r}})\right], \tag{I9a}$$

$$\nabla \times f_{l+1}(\sigma r)\mathbf{Y}_{l,l+1,1}^{m}(\Omega_{\mathbf{r}}) = j\sigma\left(\tfrac{l}{2l+1}\right)^{1/2} f_l(\sigma r)\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}), \tag{I9b}$$

$$\nabla \times f_{l-1}(\sigma r)\mathbf{Y}_{l,l-1,1}^{m}(\Omega_{\mathbf{r}}) = j\sigma\left(\tfrac{l+1}{2l+1}\right)^{1/2} f_l(\sigma r)\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}), \tag{I9c}$$

$$\nabla \times g_l(\sigma r)\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}) = -j\sigma\left[\left(\tfrac{l}{2l+1}\right)^{1/2} g_{l+1}(\sigma r)\mathbf{Y}_{l,l+1,1}^{m}(\Omega_{\mathbf{r}}) + \left(\tfrac{l+1}{2l+1}\right)^{1/2} g_{l-1}(\sigma r)\mathbf{Y}_{l,l-1,1}^{m}(\Omega_{\mathbf{r}})\right], \tag{I10a}$$

$$\nabla \times g_{l+1}(\sigma r)\mathbf{Y}_{l,l+1,1}^{m}(\Omega_{\mathbf{r}}) = -j\sigma\left(\tfrac{l}{2l+1}\right)^{1/2} g_l(\sigma r)\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}), \tag{I10b}$$

$$\nabla \times g_{l-1}(\sigma r)\mathbf{Y}_{l,l-1,1}^{m}(\Omega_{\mathbf{r}}) = -j\sigma\left(\tfrac{l+1}{2l+1}\right)^{1/2} g_l(\sigma r)\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}}). \tag{I10c}$$

The outward radial Green's function in the spherical representation is equal to [20]

$$G(\mathbf{r}-\mathbf{r}') \equiv \tfrac{1}{4\pi|\mathbf{r}-\mathbf{r}'|} e^{-\sigma|\mathbf{r}-\mathbf{r}'|} = \sigma\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_l(\sigma r_<) g_l(\sigma r_>) Y_{lm}(\Omega_{\mathbf{r}}) Y_{lm}^{*}(\Omega_{\mathbf{r}'}) \tag{I11}$$

where $r_<$ is the smallest of (r, r') and $r_>$ is the largest of (r, r').

Appendix II

Here, we shall prove the relation

$$I_{lm} \equiv \int_0^{\pi} J_m(\alpha \sin u) e^{\beta \cos u} P_l^m(\cos u) \sin u du = 2(-1)^m f_l\left(\sqrt{\beta^2 - \alpha^2}\right) P_l^m\left(\frac{\beta}{\sqrt{\beta^2 - \alpha^2}}\right), \qquad \text{(II1)}$$

where α, β are complex numbers. The modified spherical Bessel function of the first kind $f_l(z)$ for complex argument has been defined in Appendix I. The associated Legendre function $P_l^m(w)$ for complex argument w, as well as fo real argument x, is defined in Abramowitz [21].

When m=l, we have the relations

$$P_l^l(\cos u) = (-1)^l (2l-1)!!(\sin u)^l, \qquad \text{(II2a)}$$

$$P_l^l\left(\frac{\beta}{\sqrt{\beta^2 - \alpha^2}}\right) = (2l-1)!!\left(\frac{\alpha}{\sqrt{\beta^2 - \alpha^2}}\right)^l, \qquad \text{(II2b)}$$

where (2l-1)!!=1.3.5...(2l-1).

We also have the identity [22]:

$$\int_0^{\pi/2} (\sin u)^{l+1} \cosh(\beta \cos u) J_l(\alpha \sin u) du = \left(\frac{\alpha}{\sqrt{\beta^2 - \alpha^2}}\right)^l f_l\left(\sqrt{\beta^2 - \alpha^2}\right). \qquad \text{(II3)}$$

By setting $u' = \pi - u$, we obtain the relation

$$\int_{\pi/2}^{\pi} (\sin u)^{l+1} e^{\beta \cos u} J_l(\alpha \sin u) du = \int_0^{\pi/2} (\sin u')^{l+1} e^{-\beta \cos u'} J_l(\alpha \sin u') du' \qquad \text{(II4)}$$

and, therefore,

$$I_{ll} = 2(-1)^l (2l-1)!! \int_0^{\pi/2} (\sin u)^{l+1} \cosh(\beta \cos u) J_l(\alpha \sin u) du = 2(-1)^l f_l\left(\sqrt{\beta^2 - \alpha^2}\right) P_l^l\left(\frac{\beta}{\sqrt{\beta^2 - \alpha^2}}\right). \text{(II5)}$$

The relation (II1) holds for m=l.

When m=l-1, we have the relations

$$P_l^{l-1}(\cos u) = (-1)^{l-1} (2l-1)!! \cos u (\sin u)^{l-1}, \qquad \text{(II6a)}$$

$$P_l^{l-1}\left(\frac{\beta}{\sqrt{\beta^2 - \alpha^2}}\right) = (2l-1)!! \frac{\beta}{\sqrt{\beta^2 - \alpha^2}} \left(\frac{\alpha}{\sqrt{\beta^2 - \alpha^2}}\right)^{l-1}. \qquad \text{(II6b)}$$

By setting $l \to l-1$ in Eq. (II3) and taking the partial derivative with respect to β, we obtain the relation

$$\int_0^{\pi/2} \cos u(\sin u)^l \sinh(\beta\cos u) J_{l-1}(\alpha\sin u)du$$
$$= \frac{\partial}{\partial\beta}\left[f_{l-1}\left(\sqrt{\beta^2-\alpha^2}\right)\left(\frac{\alpha}{\sqrt{\beta^2-\alpha^2}}\right)^{l-1}\right] = f_l\left(\sqrt{\beta^2-\alpha^2}\right)\frac{\beta}{\sqrt{\beta^2-\alpha^2}}\left(\frac{\alpha}{\sqrt{\beta^2-\alpha^2}}\right)^{l-1}, \tag{II7}$$

where we used the identity:

$$\frac{df_{l-1}(z)}{dz} - \frac{l-1}{z} f_{l-1}(z) = f_l(z). \tag{II8}$$

The change of variable $u' = \pi - u$ leads to the relation

$$\int_{\pi/2}^{\pi} \cos u(\sin u)^l e^{\beta\cos u} J_{l-1}(\alpha\sin u)du$$
$$= -\int_0^{\pi/2} \cos u'(\sin u')^l e^{-\beta\cos u'} J_{l-1}(\alpha\sin u')du' \tag{II9}$$

and, therefore,

$$I_{l,l-1} = 2(-1)^{l-1}(2l-1)!! \int_0^{\pi/2} \cos u(\sin u)^l \sinh(\beta\cos u) J_{l-1}(\alpha\sin u)du$$
$$= 2(-1)^{l-1} f_l\left(\sqrt{\beta^2-\alpha^2}\right) P_l^{l-1}\left(\frac{\beta}{\sqrt{\beta^2-\alpha^2}}\right). \tag{II10}$$

We have shown that the relation (II1) holds for m=l, l-1. Next, we shall show that, if it is true for (l-1,m) and (l-2,m), then it is true to (l,m). Therefore, by induction, it is true for m=l-2, l-1, …, 1,0. For this purpose, we use the identity [23]:

$$P_l^m(z) = \frac{2l-1}{l-m} zP_{l-1}^m(z) - \frac{l+m-1}{l-m} P_{l-2}^m(z). \tag{II11}$$

Substitution of this identity into Eq. (II1) gives the relation

$$I_{l,m} = \frac{2l-1}{l-m}\frac{\partial}{\partial\beta} I_{l-1,m} - \frac{l+m-1}{l-m} I_{l-2,m}$$
$$= 2(-1)^m\left[\frac{2l-1}{l-m}\frac{\partial}{\partial\beta}\left(P_{l-1}^m\left(\frac{\beta}{\sqrt{\beta^2-\alpha^2}}\right) f_{l-1}\left(\sqrt{\beta^2-\alpha^2}\right)\right) - \frac{l+m-1}{l-m} P_{l-2}^m\left(\frac{\beta}{\sqrt{\beta^2-\alpha^2}}\right) f_{l-2}\left(\sqrt{\beta^2\alpha^2}\right)\right]. \tag{II12}$$

Here, we have assumed that Eq. (II1) is valid for (l-1,m) and (l-2,m). After taking the partial derivative and using the identity (II8), as well as, the identity:

$$\left(z^2-1\right)\frac{dP_l^m(z)}{dz} = (l-m+1)P_{l+1}^m(z) - (l+1)zP_l^m(z), \tag{II13}$$

we obtain the relation:

$$I_{l,m} = \frac{2(-1)^m}{l-m}\left\{ f_l\left[(2l-1)\frac{\beta}{\sqrt{\beta^2-\alpha^2}}P_{l-1}^m - (l+m-1)P_{l-2}^m\right]\right.$$

$$\left. + (2l-1)\frac{1}{\sqrt{\beta^2-\alpha^2}} f_{l-1}\left[(2l-1)\frac{\beta}{\sqrt{\beta^2-\alpha^2}}P_{l-1}^m - (l+m-1)P_{l-2}^m - (l-m)P_l^m\right]\right\}, \tag{II14}$$

where the arguments of f_l, P_l^m are given above. The identity

$$(2l-1)zP_{l-1}^m(z) = (l-m)P_l^m(z) + (l+m-1)P_{l-2}^m(z), \tag{II14a}$$

applied to the relation above, leads to the validity of Eq. (II1).

When we set $\alpha = k_\rho r, \beta = -\gamma_2 r$, where $\gamma_2 = \left[k_\rho^2 + \sigma_2^2\right]^{1/2}$, Eq. (II1) becomes equal to

$$\int_0^\pi J_m(k_\rho r \sin u) e^{-\gamma_2 r \cos u} P_l^m(\cos u) \sin u\, du$$

$$= 2(-1)^l P_l^m\left(\frac{\gamma_2}{\sigma_2}\right) f_l(\sigma_2 r), \tag{II15}$$

where

$$P_l^m\left(\frac{\gamma_2}{\sigma_2}\right) = \left(\frac{k_\rho}{\sigma_2}\right)^m \left.\frac{d^m P_l(w)}{dw^m}\right|_{w=\frac{\gamma_2}{\sigma_2}}, \tag{II16a}$$

when $m \geq 0$, and

$$P_l^m\left(\frac{\gamma_2}{\sigma_2}\right) = \frac{(l-|m|)!}{(l+|m|)!} P_l^{|m|}\left(\frac{\gamma_2}{\sigma_2}\right) \tag{II16b}$$

when $m<0$. In Eqs. (II15) we used the identity

$$P_l^m(-w) = (-1)^{l-m} P_l^m(w). \tag{II17}$$

Finally, we use the identity

$$e^{-j\mathbf{k}_\rho \cdot \boldsymbol{\rho}} = \sum_{m=-\infty}^{\infty} (-j)^m J_m(k_\rho \rho) e^{-jm(\varphi - \varphi_k)}. \tag{II18}$$

where (ρ, φ) and (k_ρ, φ_k) are the cylindrical coordinates of the vectors $\boldsymbol{\rho}$ and $\mathbf{k}_\rho$, respectively. With the help of this identity, of Eq. (II15) and the completeness and orthonormality of the scalar spherical harmonics it is a simple matter to prove the identity

$$e^{-j\mathbf{k}_\rho \cdot \boldsymbol{\rho} - \gamma_2 z} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (-1)^l f_l(\sigma_2 r) Y_{lm}^*(\Omega_r) \tilde{Y}_{lm}\left(\frac{\gamma_2}{\sigma_2}, \varphi_k\right) \tag{II19}$$

where σ_2 is a complex number. The complex scalar spherical harmonics are defined as follows:

$$\tilde{Y}_{lm}\left(\frac{\gamma_2}{\sigma_2}, \varphi_k\right) = (-j)^m \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l-m)!}\right]^{1/2} P_l^m\left(\frac{\gamma_2}{\sigma_2}\right) e^{jm\varphi_k}, \tag{II20}$$

where $P_l^m\left(\frac{\gamma_2}{\sigma_2}\right)$ is given by Eqs. (16a), (16b). Notice that $P_l^m(z)$ is zero when $|m| > l$. If the real part of σ_2 tends to zero, i.e., medium 2 is non-absorptive, then $\widetilde{Y}_{lm}$ reduces to the usual scalar spherical harmonics and Eq. (II19) reduces to the usual expansion of $\exp(-j\mathbf{k}\cdot\mathbf{r})$ in terms of spherical harmonics.

Appendix III

We define:

$$f_{lm}(\rho,|z|) = (-1)^m \int_0^\infty J_m(\lambda\rho) e^{-\gamma|z|} P_l^m\left(\frac{\gamma}{\sigma}\right)\frac{\lambda d\lambda}{\sigma\gamma} \qquad \text{(III1)}$$

where

$$\gamma = \left[\lambda^2 + \sigma^2\right]^{1/2}. \qquad \text{(III2)}$$

Also we define

$$\tilde{f}_{lm}(\rho,|z|) = g_l(\sigma r) P_l^m\left(\frac{|z|}{r}\right) \qquad \text{(III3)}$$

where

$$r = \left[\rho^2 + z^2\right]^{1/2}. \qquad \text{(III4)}$$

We shall prove that

$$f_{lm}(\rho,|z|) = \tilde{f}_{lm}(\rho,|z|). \qquad \text{(III5)}$$

Here, σ is a complex number with a positive real part, i.e., $\sigma_r > 0$.

A) From the identity (w a real or complex number) [23]:

$$P_{l+1}^m(w) = \frac{1}{l-m+1}\left[(2l+1)wP_l^m(w) - (l+m)P_{l-1}^m(w)\right], \qquad \text{(III6)}$$

it follows immediately that

$$f_{l+1,m} = \frac{1}{l-m+1}\left[(2l+1)\left(-\frac{1}{\sigma}\frac{\partial}{\partial|z|}\right)f_{lm} - (l+m)f_{l-1,m}\right]. \qquad \text{(III7)}$$

We shall prove that $\tilde{f}_{lm}$ satisfies this identity too. We have

$$\frac{1}{\sigma}\frac{\partial}{\partial|z|}\tilde{f}_{lm} = \frac{|z|}{r}g_l'(\sigma r)P_l^m\left(\frac{|z|}{r}\right) + \frac{1}{\sigma r}g_l(\sigma r)\left[1 - \left(\frac{z}{r}\right)^2\right]P_l^{m\prime}\left(\frac{|z|}{r}\right). \qquad \text{(III8)}$$

We use the identity ($|x|<1$, real)

$$\left[1 - x^2\right]P_l^{m\prime}(x) = -\frac{(l-m+1)}{2l+1}P_{l+1}^m(x) + \frac{(l+m)(l+1)}{2l+1}P_{l-1}^m(x). \qquad \text{(III9)}$$

Then

$$-(2l+1)\frac{1}{\sigma}\frac{\partial}{\partial|z|}\tilde{f}_{lm} - (l+m)\tilde{f}_{l-1,m} = -(2l+1)\frac{|z|}{r}g_l' P_l^m - (l+m)\left[g_{l-1} + \frac{l+1}{\sigma r}g_l\right]$$
$$+ (l-m+1)l\frac{1}{\sigma r}g_l P_{l+1}^m. \qquad \text{(III10)}$$

We use the identities

$$g_{l-1} + \frac{l+1}{\sigma r}g_l = -g_l', \qquad \text{(III11a)}$$

$$\tfrac{1}{\sigma r} g_l = g_l' \;\; + g_{l+1}. \tag{III11b}$$

Then

$$\begin{aligned}&(2l+1)\left(-\tfrac{1}{\sigma}\tfrac{\partial}{\partial|z|}\right)\tilde{f}_{lm} - (l+m)\tilde{f}_{l-1,m}\\ &= (l-m+1)\tilde{f}_{l+1,m} + g_l' \left[-(2l+1)\tfrac{|z|}{r} P_l^m + (l-m+1)P_{l+1}^m + (l+m)P_{l-1}^m\right]\end{aligned} \tag{III12}$$

From the identity (III6) it follows immediately that $\tilde{f}_{lm}$ satisfies Eq. (III7) as well.

B) From the identity (|x|<1, real)

$$P_l^{m+2}(x) + 2(m+1)\tfrac{x}{\sqrt{1-x^2}} P_l^m(x) + (l-m)(l+m+1)P_l^m(x) = 0\,, \tag{III13}$$

it follows immediately that

$$\tilde{f}_{l,m+2} = -2(m+1)\tfrac{|z|}{\rho}\tilde{f}_{l,m+1} - (l-m)(l+m+1)\tilde{f}_{lm}\,. \tag{III14}$$

We shall prove that f_{lm} satisfies this identity too.

From the definition of f_{lm} we have:

$$\begin{aligned}(-1)^{m+1}|z| f_{l,m+1} &= -\int_0^\infty J_{m+1}(\lambda p)\left[\tfrac{\partial}{\partial\lambda} e^{-\gamma|z|}\right] P_l^{m+1}\left(\tfrac{\gamma}{\sigma}\right)\tfrac{d\lambda}{\sigma}\\ &= \int_0^\infty \left[\rho J_{m+1}'(\lambda\rho) P_l^{m+1}\left(\tfrac{\gamma}{\sigma}\right) + \tfrac{\lambda}{\sigma\gamma} J_{m+1}(\lambda\rho) P_l^{m'}\left(\tfrac{\gamma}{\sigma}\right)\right] e^{-\gamma|z|}\tfrac{d\lambda}{\sigma},\end{aligned} \tag{III15}$$

We use the identities [23-24]:

$$J_{m+1}'(\lambda\rho) = -(m+1)J_{m+1}(\lambda\rho) + \lambda\rho J_m(\lambda\rho), \tag{III16a}$$

$$\left(w^2-1\right)P_l^{m+1'}(w) - (m+1)wP_l^{m+1}(w) = \sqrt{w^2-1}\,P_l^{m+2}(w). \tag{III16b}$$

Then

$$-2(m+1)\tfrac{|z|}{\rho} f_{l,m+1} = 2(m+1)(-1)^m \int_0^\infty \left[J_m(\lambda\rho)\tfrac{\gamma}{\lambda}P_l^{m+1}\left(\tfrac{\gamma}{\sigma}\right) + \tfrac{1}{\lambda\rho}J_{m+1}P_l^{m+1}\left(\tfrac{\gamma}{\sigma}\right)\right] e^{-\gamma|z|}\tfrac{\lambda d\lambda}{\gamma\sigma}. \tag{III17}$$

We use the identities [23-24]:

$$J_{m+2}(\lambda\rho) = -J_m(\lambda\rho) + \tfrac{2(m+1)}{\lambda\rho} J_{m+1}(\lambda\rho), \tag{III18a}$$

$$P_l^{m+2}(w) - (l-m)(l+m+1)P_l^m(w) = -2(m+1)\tfrac{w}{\sqrt{w^2-1}} P_l^{m+1}(w). \tag{III18b}$$

Then:

$$\begin{aligned}&J_{m+2}(\lambda\rho)P_l^{m+2}\left(\tfrac{\gamma}{\sigma}\right) + (l-m)(l+m+1)J_m(\lambda\rho)P_l^m\left(\tfrac{\gamma}{\sigma}\right)\\ &= 2(m+1)\left[J_m(\lambda\rho)\tfrac{\gamma}{\lambda}P_l^{m+1}\left(\tfrac{\gamma}{\sigma}\right) + \tfrac{1}{\lambda\rho}J_m(\lambda\rho)P_l^{m+2}\left(\tfrac{\gamma}{\sigma}\right)\right]\end{aligned}\,. \tag{III19}$$

Substitution of this identity into Eq. (III17) leads to the relation we want to prove, namely, f_{lm} satisfies also the identity (III14).

C) We have proved that both f_{lm} and $\tilde{f}_{lm}$ satisfy the identities given by Eqs. (III7), (III14). If f_{00}, f_{11} are known, all the other f_{lm} for l=1,2,3,... and m=-l, -l+1, ..., l-1, l can be computed from these two identities. Therefore, if we show that

$$f_{00}(\rho,|z|) = \tilde{f}_{00}(\rho,|z|), \tag{III20a}$$

$$f_{11}(\rho,|z|) = \tilde{f}_{11}(\rho,|z|), \tag{III20b}$$

then we have proven the validity of Eq. (III5). Eq. (III20a) is tabulated in I.S. Gradshteyn and I.M. Ryzhik [25]. Notice that this relation is valid only when the real part of σ is greater than zero. Eq. (III20b) follows from Eq. (III20a) by differentiating the latter with respect to ρ.

From the identity

$$e^{-j\lambda\cdot\rho} = \sum_{m=-\infty}^{\infty}(-j)^m J_m(\lambda\rho)e^{jm(\varphi-\varphi_\lambda)}, \tag{III21}$$

we obtain the relation

$$\int_0^{2\pi} e^{-j\lambda\cdot\rho+jm\varphi_\lambda}\,d\varphi_\lambda = 2\pi(-j)^m J_m(\lambda\rho)e^{jm\varphi}\,. \tag{III22}$$

Combining Eqs. (III5), (III22) with the definitions of $Y_{lm}(\Omega_r)$ and the complex scalar spherical harmonics $\tilde{Y}_{lm}(\gamma/\sigma,\varphi_\lambda)$ (cf. Eq. II19), we obtain the following useful identity:

$$g_l(\sigma r)Y_{lm}(\Omega_r) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\tilde{Y}_{lm}\left((\mathrm{sign}z)\frac{\gamma}{\sigma},\varphi_\lambda\right)e^{-j\lambda\cdot\rho-\gamma|z|}\frac{d\lambda_x d\lambda_y}{\gamma\sigma}, \tag{III23}$$

where

$$\mathrm{sign}z = \begin{matrix} 1 \text{ if } z>0 \\ -1 \text{ if } z<0 \end{matrix}. \tag{III24}$$

Appendix IV

Here, we shall prove the scalar addition theorem, namely, the identity;

$$g_l(\sigma|\mathbf{r}-\mathbf{r}_0|)Y_{lm}(\Omega_{r-r_0}) = \sum_{l''=0}^{\infty}\sum_{m''=l''}^{l''}\widetilde{G}_{lm;l''m''}(\mathbf{r}_0)f_{l''}(\sigma r)Y_{l''m''}(\Omega_r) \tag{IV1}$$

where σ is a complex number with a positive real part, $r_0>r$, and

$$\widetilde{G}_{lm;l''m''}(\mathbf{r}_0) = 4\pi(-1)^{l-m}\sum_{l'm'}B_{lm}(l'm';l''m'')g_l(\sigma r_0)Y_{l',-m'}(\Omega_{r_0}). \tag{IV2}$$

The quantity $B_{lm}(l'm';l''m'')$ in terms of the Wigner 3j-symbol is equal to [26]:

$$B_{lm}(l'm';l''m'') = \left[\frac{(2l+1)(2l'+1)(2l''+1)}{4\pi}\right]^{1/2} * \begin{pmatrix} l\, l''\, l' \\ 0\,0\,0 \end{pmatrix}\begin{pmatrix} l & l'' & l' \\ m- & m'' & m' \end{pmatrix}. \tag{IV3}$$

Since $B_{lm}(l'm';l''m'')$ is different from zero only when $l' = |l-l''|, |l-l''|+1, ..., l+l''$, and $m' = m'' - m$, the sum over (l', m') in Eq. (IV2) extends only over these values.

When $m\geq 0$, from the identity (III24), we obtain in operator form the relation (cf. Eq. II16a)

$$g_l(\sigma r)Y_{lm}(\Omega_r) = \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^{(m)}\left(-\frac{1}{\sigma}\frac{\partial}{\partial z}\right)\left(\frac{1}{\sigma}\frac{\partial}{\partial x} + j\frac{1}{\sigma}\frac{\partial}{\partial y}\right)^m g_0(\sigma r), \tag{IV4a}$$

where

$$P_l^{(m)}(w) = \frac{d^m P_l(w)}{dw^m} \tag{IV4b}$$

If we use the usual addition theorem when $r_0>r$, namely,

$$g_0(\sigma|\mathbf{r}-\mathbf{r}_0|) = 4\pi\sum_{l''=0}^{\infty}\sum_{m''=-l''}^{l''}(-1)^{m''}f_{l''}(\sigma r)g_{l''}(\sigma r_0)Y_{l''m''}(\Omega_r)Y_{l'',-m''}(\Omega_{r_0}), \tag{IV5}$$

then Eq. (IV4) yields the relation in Eq. (IV1), where

$$\widetilde{G}_{lm;l''m''}(\mathbf{r}_0) = \left[\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2}(-1)^{m+m''}P_l^{(m)}\left(\frac{1}{\sigma}\frac{\partial}{\partial z_0}\right)\left(\frac{1}{\sigma}\frac{\partial}{\partial x_0} + j\frac{1}{\sigma}\frac{\partial}{\partial y_0}\right)^m g_{l''}(\sigma r_0)Y_{l'',-m''}(\Omega_{r_0}) \tag{IV6}$$

If we use again the identity (III24) and perform the differentiations as prescribed in Eq. (IV6), we obtain the relation

$$\widetilde{G}_{lm;l''m}(\mathbf{r}_0) = 4\pi(-1)^{l+m''}(\mathrm{sign} z_0)^{l-m+l''-m''} * \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\widetilde{Y}_{lm}\left(\frac{\gamma}{\sigma},\varphi_\lambda\right)\widetilde{Y}_{l'',-m''}\left(\frac{\gamma}{\sigma},\varphi_\lambda\right)e^{-j\lambda\cdot\rho_0-\gamma|z_0|}\frac{d\lambda_x d\lambda_y}{\gamma\sigma} \tag{IV7}$$

The product of the complex spherical harmonics in Eq. (IV7) can be written as the sum of complex spherical harmonics, namely,

$$\widetilde{Y}_{lm}\left(\tfrac{\gamma}{\sigma},\varphi_\lambda\right)\widetilde{Y}_{l'',-m''}\left(\tfrac{\gamma}{\sigma},\varphi_\lambda\right)=\sum_{l'm'}(-1)^{m'}B_{lm}(l'm';l''m'')\widetilde{Y}_{l',-m'}\left(\tfrac{\gamma}{\sigma},\varphi_\lambda\right) \tag{IV8}$$

When the real part of σ tends to zero, then the complex spherical harmonics become the usual real spherical harmonics and $B_{lm}(l'm';l''m'')$ is given by Eq. (IV3). The sum is extended over $l'=|l-l''|,|l-l''|+1,\ldots,l+l''$, and $m'=m''-m$. Only for those values $B_{lm}(l'm';l''m'')$ is different from zero. When $w=\gamma/\sigma$ is a complex variable, then Eq. (IV8) expresses really an identity between the product of two polynomials and the sum of a set of polynomials. The coefficients $(-1)^{m'}B_{lm}(l'm';l''m'')$ in the sum are the same for any value of w. Therefore, if Eq. (IV8) is valid for real w less than one, it is also valid for complex w.

Substitution of Eq. (IV8) into Eq. (IV7) and use of the identity (III24) yields the relation

$$\widetilde{G}_{lm;l''m''}(\mathbf{r}_0)=4\pi(-1)^{l-m}\sum_{l'm'}(\mathrm{sign}z_0)^{l-m+l'-m'+l''-m''}B_{lm}(l'm';l''m'')g_{l'}(\sigma r_0)Y_{l',-m'}(\Omega_{r0}) \tag{IV9}$$

where we used the fact that $m'=m''-m$. Notice that $B_{lm}(l'm';l''m'')$ is different from zero only when $l'=l-l''+2n$, for $l\geq l''$, where $n=0,1,\ldots,l''$, and only when $l'=l''-l+2n$, for $l''>l$, where n=0,1,…,l. Therefore, $l+l'+l''$ and $m+m'+m''$ are even integers and Eq. (IV9) becomes identical to Eq. (IV2).

The function $\widetilde{G}_{lm;l'm'}(\mathbf{r}_0)$ can be written in integral form rather easily. Multiply Eq. (IV1) by $f^*_{l'}(\sigma r)Y^*_{l'm'}(\Omega_r)$ and integrate over the volume V_0 of the sphere. Due to the orthonormality of the spherical harmonics, we obtain the relation

$$\widetilde{G}_{lm;l'm'}(\mathbf{r}_0)=\frac{1}{\zeta_{l'}}\int_{V_0} g_l(\sigma|\mathbf{r}-\mathbf{r}_0|)Y_{lm}(\Omega_{r-r0})f^*_{l'}(\sigma r)Y^*_{l'm'}(\Omega r)d^3x \tag{IV10}$$

where ζ_l is given by Eq. (56).

Appendix V

Here, we shall prove the vector addition theorem, namely, the identity:

$$g_\ell\left(\sigma\left|\mathbf{r}-\mathbf{r}_0\right|\right)\mathbf{Y}^{m}_{\ell\ell 1}\left(\Omega_{r-r_0}\right)$$
$$=\sum_{\ell'=1}^{\infty}\sum_{m'=-\ell'}^{l'}\Big[\widetilde{U}_{lm;l'm'}(\mathbf{r}_0)f_{\ell'}(\sigma r)\mathbf{Y}^{m'}_{\ell'\ell'1}(\Omega_{\mathbf{r}}) \tag{V1}$$
$$+\widetilde{V}_{\ell m;\ell' m'}(\mathbf{r}_0)\tfrac{1}{j\sigma}\left(f_{\ell'}(\sigma r)\mathbf{Y}^{m'}_{\ell'\ell'1}(\Omega_{\mathbf{r}})\right)+\tfrac{1}{\sigma}\widetilde{W}_{\ell m;\ell' m'}(\mathbf{r}_0)\nabla\left(f_{\ell'}(\sigma r)Y_{\ell' m'}(\Omega_{\mathbf{r}})\right)\Big]$$

where σ is a complex number with positive real part, $r_0 > r$, and

$$\widetilde{U}_{lm;l'm'}(\mathbf{r}_0)=\frac{1}{[l(l+1)l'(l'+1)]^{1/2}}$$
$$*\left[2\alpha_l^m\beta_{l'}^{m'+1}\widetilde{G}_{l,m+1;l',m'+1}(\mathbf{r}_0)+2\alpha_{l'}^{m'-1}\beta_l^m\widetilde{G}_{l,m-1;l',m'-1}(\mathbf{r}_0)+mm'\widetilde{G}_{lm;l'm'}(\mathbf{r}_0)\right], \tag{V2a}$$

$$\widetilde{V}_{lm;l'm'}(\mathbf{r}_0)=\frac{2l'+1}{[l(l+1)l'(l'+1)]^{1/2}}(-1)^{m'}\sqrt{\frac{4\pi}{3}}$$
$$*\Big[\sqrt{2}\alpha_l^m B_{l'-1,m'+1}(1,-1;l'm')\widetilde{G}_{l,m+1;l'-1,m'+1}(\mathbf{r}_0)-\sqrt{2}\beta_l^m B_{l'-1,m'-1}(1,1;l'm')\widetilde{G}_{l,m-1;l'-1,m-1}(\mathbf{r}_0) \tag{V2b}$$
$$+mB_{l'-1,m'}(1,0;l'm')\widetilde{G}_{l,m;l'-1,m'}(\mathbf{r}_0)\Big],$$

$$\widetilde{W}_{lm;l'm'}(\mathbf{r}_0)=0 \tag{V2c}$$

Also, α_l^m and β_l^m are given by Eqs. (37a), (37b) while $\widetilde{G}_{lm;l'm'}(r_0)$ is given by Eq. (IV2).

A) First, we shall compute $\widetilde{U}_{lm;l'm'}(\mathbf{r}_0)$. Applying the curl on Eq. (V1), we obtain the relation

$$\tfrac{1}{j\sigma}\nabla\times\left(g_l\left(\sigma\left|\mathbf{r}-\mathbf{r}_0\right|\right)\mathbf{Y}^m_{lll}\left(\Omega_{r-r_0}\right)\right)$$
$$=\sum_{l'm'}\left[\widetilde{V}_{lm;l'm'}(\mathbf{r}_0)f_{l'}(\sigma r)\mathbf{Y}^{m'}_{l'l'1}(\Omega_{\mathbf{r}})+\widetilde{U}_{lm;l'm'}(\mathbf{r}_0)\tfrac{1}{j\sigma}\nabla\times\left(f_{l'}(\sigma r)\mathbf{Y}^{m'}_{l'l'1}(\Omega_{\mathbf{r}})\right)\right]. \tag{V3}$$

Use of the identity

$$\mathbf{L}\cdot\mathbf{F}(\mathbf{r})=-j\mathbf{r}\cdot\nabla\times\mathbf{F}(\mathbf{r}) \tag{V4}$$

where $\mathbf{L}=-j\mathbf{r}\times\nabla$ and $\mathbf{F}(\mathbf{r})$ is any vector function, together with Eq. (I4a) leads to the relation

$$\mathbf{L}\cdot\left(g_l\left(\sigma\left|\mathbf{r}-\mathbf{r}_0\right|\right)\mathbf{Y}^m_{lll}\left(\Omega_{r-r_0}\right)\right)$$
$$=\sum_{l'm'}\widetilde{U}_{lm;l'm'}(\mathbf{r}_0)(-j)\mathbf{r}\cdot\nabla\times\left(f_{l'}(\sigma r)\mathbf{Y}^{m'}_{l'l'1}(\Omega_{\mathbf{r}})\right). \tag{V5}$$

Using again the identity (V4) and Eq. (I1a) it follows that

$$-j\mathbf{r}\cdot\nabla\left(f_{l'}(\sigma r)\mathbf{Y}^{m'}_{l'l'1}(\Omega_{\mathbf{r}})\right)=\frac{1}{[l'(l'+1)]^{1/2}}\mathbf{L}\cdot\mathbf{L}\left(f_{l'}(\sigma r)Y_{l'm'}(\Omega_{\mathbf{r}})\right)=[l'(l'+1)]^{1/2}f_{l'}(\sigma r)Y_{l'm'}(\Omega_{\mathbf{r}}). \tag{V6}$$

Then, substitution of Eq. (V6) into Eq. (V5) yields the relation

$$\begin{aligned}&\mathbf{L}\cdot\left(g_l\left(\sigma\left|\mathbf{r}-\mathbf{r}_0\right|\right)\mathbf{Y}_{lll}^m\left(\Omega_{r-r0}\right)\right)\\&=\sum_{l'm'}\left[l'(l'+1)\right]^{1/2}\widetilde{U}_{lm;l'm'}(\mathbf{r}_0)f_{l'}(\sigma r)Y_{l'm'}(\Omega_r).\end{aligned}\tag{V7}$$

On the other hand, from the definition of $\mathbf{Y}_{lll}^m(\Omega\mathbf{r})$ (of Eq. (I1a) and the identifies:

$$L_+Y_{lm}(\Omega_r)=2\alpha_l^mY_{l,m+1}(\Omega_r),\tag{V8a}$$

$$L_-Y_{lm}(\Omega_r)=2\beta_l^mY_{l,m-1}(\Omega_r),\tag{V8b}$$

$$L_zY_{lm}(\Omega_r)=mY_{lm}(\Omega_r),\tag{V8c}$$

where $L_\pm=L_x\pm jL_y$ and α_l^m,β_l^m are given by Eqs. (37a) and (37b),we obtain the relation

$$\begin{aligned}&\left[l(l+1)\right]^{1/2}\mathbf{Y}_{lll}^m\left(\Omega_{r-r0}\right)\\&=\left[\alpha_l^mY_{l,m+1}\left(\Omega_{r-r0}\right)+\beta_l^mY_{l,m-1}\left(\Omega_{r-r0}\right)\right]\mathbf{e}_x\\&-j\left[\alpha_l^mY_{l,m+1}\left(\Omega_{r-r0}\right)-\beta_l^mY_{l,m-1}\left(\Omega_{r-r0}\right)\right]\mathbf{e}_y+mY_{lm}\left(\Omega_{r-r0}\right)\mathbf{e}_z\end{aligned}\tag{V9}$$

Multiply Eq. (V9) by $g_l(\sigma|\mathbf{r}-\mathbf{r}_0|)$ and apply the scalar addition theorem, i.e., Eq. (IV1). We obtain the relation

$$\begin{aligned}&\left[l(l+1)\right]^{1/2}g_l\left(\sigma\left|\mathbf{r}-\mathbf{r}_0\right|\right)\mathbf{Y}_{lll}^m\left(\Omega_{r-r0}\right)\\&=\sum_{l'm'}\Big\{\left[\alpha_l^m\widetilde{G}_{l,m+1;l'm'}(\mathbf{r}_0)+\beta_l^m\widetilde{G}_{l,m-1;l'm'}(\mathbf{r}_0)\right]\mathbf{e}_x\\&-j\left[\alpha_l^m\widetilde{G}_{l,m+1;l'm'}(\mathbf{r}_0)-\beta_l^m\widetilde{G}_{l,m-1;l'm'}(\mathbf{r}_0)\right]\mathbf{e}_y+m\widetilde{G}_{lm;l'm'}(\mathbf{r}_0)\mathbf{e}_z\Big\}f_{l'}(\sigma r)Y_{l'm'}(\Omega_r).\end{aligned}\tag{V10}$$

Apply the operator $\mathbf{L}$ on Eq. (V10) and use Eqs. (V8a) – (V8c). We obtain the relation

$$\begin{aligned}&\left[l(l+1)\right]^{1/2}\mathbf{L}\cdot\left(g_l\left(\sigma\left|\mathbf{r}-\mathbf{r}_0\right|\right)\mathbf{Y}_{lll}^m\left(\Omega_{r-r0}\right)\right)\\&=\sum_{l'm'}\Big[2\alpha_l^m\beta_{l'}^{m'+1}\widetilde{G}_{l,m+1;l',m'+1}(\mathbf{r}_0)\\&+2\alpha_{l'}^{m'-1}\beta_l^m\widetilde{G}_{l,m-1;l',m'-1}(\mathbf{r}_0)+mm'\widetilde{G}_{lm;l'm'}(\mathbf{r}_0)\Big]f_{l'}(\sigma r)Y_{l'm'}(\Omega_r)\end{aligned}\tag{V11}$$

Eq. (V2a) follows directly from Eqs. (V7), (V11) and the completeness of the spherical harmonics.

B) Next we shall compute $\widetilde{V}_{lm;l'm'}(\mathbf{r}_0)$. From Eqs. (V1) and (V6) we obtain the relation

$$\begin{aligned}&g_l\left(\sigma\left|\mathbf{r}-\mathbf{r}_0\right|\right)\mathbf{r}\cdot\mathbf{Y}_{lll}^m\left(\Omega_{r-r0}\right)\\&=\sum_{l'm'}\left[\widetilde{V}_{lm;l'm'}(\mathbf{r}_0)\tfrac{1}{\sigma}\left[l'(l'+1)\right]^{1/2}f_{l'}(\sigma r)Y_{l'm'}(\Omega_r)+\widetilde{W}_{lm;l'm'}(\mathbf{r}_0)rf'_{l'}(\sigma r)Y_{l'm'}(\Omega_r)\right].\end{aligned}\tag{V12}$$

On the other hand, from Eq. (V10) we obtain the relation

$$
\begin{aligned}
&[l(l+1)]^{1/2} g_l(\sigma|\mathbf{r}-\mathbf{r}_0|)\mathbf{r}\cdot\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}-\mathbf{r}0})\\
&=\sum_{l'm'}\Big[\alpha_l^m\widetilde{G}_{l,m+1;l'm'}(\mathbf{r}_0)(x-jy)f_{l'}(\sigma r)Y_{l'm'}(\Omega_r)\\
&+\beta_l^m\widetilde{G}_{l,m-1;l'm'}(\mathbf{r}_0)(x+jy)f_{l'}(\sigma r)Y_{l'm'}(\Omega_r)+m\widetilde{G}_{lm;l'm'}(\mathbf{r}_0)zf_{l'}(\sigma r)Y_{l'm'}(\Omega_r)\Big].
\end{aligned}
\tag{V13}
$$

Substitute the relations

$$x\pm jy=\mp\sqrt{\tfrac{8\pi}{3}}\,rY_{1,\pm1}(\Omega_r), \tag{V14a}$$

$$z=\sqrt{\tfrac{4\pi}{3}}\,rY_{10}(\Omega_r) \tag{V14b}$$

into Eq. (V13) and replace the products of the spherical harmonics by means of Eq. (IV8) for real γ/σ. Then Eq. (V13) becomes equal to

$$
\begin{aligned}
&[l(l+1)]^{1/2} g_l(\sigma|\mathbf{r}-\mathbf{r}_0|)\mathbf{r}\cdot\mathbf{Y}_{lll}^{m}(\Omega_{\mathbf{r}-\mathbf{r}0})\\
&=\sum_{l'm'}\big[A_{lm;l'm'}(\mathbf{r}_0)rf'_{l+1}(\sigma r)+B_{lm;l'm'}(\mathbf{r}_0)rf_{l'-1}(\sigma r)\big]Y_{l'm'}(\Omega_r),
\end{aligned}
\tag{V15}
$$

where

$$
\begin{aligned}
&A_{lm;l'm'}(\mathbf{r}_0)=(-1)^{m'}\sqrt{\tfrac{4\pi}{3}}\\
&*\Big[\sqrt{2}\alpha_l^m\widetilde{G}_{l,m+1;l'+1,m'+1}(\mathbf{r}_0)B_{l'+1,m'+1}(1,-1;l'm')\\
&-\sqrt{2}\beta_l^m\widetilde{G}_{l,m-1;l'+1,m'-1}(\mathbf{r}_0)B_{l'+1,m'-1}(1,1;l'-m')\\
&+m\widetilde{G}_{lm;l'+1,m'}B_{l'+1,m'}(1,0;l'm')\Big],
\end{aligned}
\tag{V16a}
$$

$$
\begin{aligned}
&B_{lm;l'm'}(\mathbf{r}_0)=(-1)^{m'}\sqrt{\tfrac{4\pi}{3}}\\
&*\Big[\sqrt{2}\alpha_l^m\widetilde{G}_{l,m+1;l'-1,m'+1}(\mathbf{r}_0)B_{l'-1,m'+1}(1,-1;l'm')\\
&-\sqrt{2}\beta_l^m\widetilde{G}_{l,m-1;l'-1,m'-1}(\mathbf{r}_0)B_{l'-1,m'-1}(1,1;l'-m')\\
&+m\widetilde{G}_{lm;l'-1,m'}B_{l'-1,m'}(1,0;l'm')\Big].
\end{aligned}
\tag{V16b}
$$

Substitute the relations

$$\sigma rf_{l'+1}(\sigma r)=\sigma rf'_{l'}(\sigma r)-l'f_{l'}(\sigma r), \tag{V17a}$$

$$\sigma rf_{l'-1}(\sigma r)=\sigma rf'_{l'}(\sigma r)+(l'+1)f_{l'}(\sigma r), \tag{V17b}$$

into Eq. (V15). Then from Eqs. (V12), (V15) and the completeness of the spherical harmonics, we obtain the relation

$$\widetilde{A}_{lm;l'm'}(\mathbf{r}_0)f_{l'}(\sigma r)+\widetilde{B}_{lm;l'm'}(\mathbf{r}_0)\sigma rf'_{l}(\sigma r)=0, \tag{V18}$$

where

$$\widetilde{A}_{lm;l'm'}(\mathbf{r}_0)=[l(l+1)l'(l'+1)]^{1/2}\widetilde{V}_{lm;l'm'}(\mathbf{r}_0)+l'A_{lm;l'm'}(\mathbf{r}_0)-(l'+1)B_{lm;l'm'}(\mathbf{r}_0), \tag{V19a}$$

$$\widetilde{B}_{lm;l'm'}(\mathbf{r}_0) = [l(l+1)]^{1/2}\, \widetilde{W}_{lm;l'm'}(\mathbf{r}_0) - A_{lm;l'm'}(\mathbf{r}_0) - B_{lm;l'm'}(\mathbf{r}_0). \tag{V19b}$$

Equ. (V18) is valid for all values of r. Since there is at least one pair of values (z_1, z_2), where $z_1=\sigma r_1$, $z_2=\sigma r_2$, for which the determinant

$$D = \begin{vmatrix} f_{l'}(z_1) & z_1 f'_{l'}(z_1) \\ f_{l'}(z_2) & z_2 f'_{l'}(z_2) \end{vmatrix}$$

is different from zero, we conclude that:

$$\widetilde{A}_{lm;l'm'}(\mathbf{r}_0) = \widetilde{B}_{lm;l'm'}(\mathbf{r}_0) = 0\,, \tag{V20}$$

and, therefore, we have the relations

$$\widetilde{V}_{lm;l'm'}(\mathbf{r}_0) = \frac{1}{[l(l+1)l'(l'+1)]^{1/2}}\left[-l'A_{lm;l'm'}(\mathbf{r}_0) + (l'+1)B_{lm;l'm'}(\mathbf{r}_0)\right], \tag{V21a}$$

$$\widetilde{W}_{lm;l'm'}(\mathbf{r}_0) = \frac{1}{[l(l+1)]^{1/2}}\left[A_{lm;l'm'}(\mathbf{r}_0) + B_{lm;l'm'}(\mathbf{r}_0)\right]. \tag{V21b}$$

C) From Eq. (I4a) and the identity $\nabla\cdot(\mathbf{L}Y_{lm}) = 0$, where $\mathbf{L} = -j\mathbf{r}\times\nabla$, we obtain that relation

$$\nabla\cdot\left(h(\sigma r)\mathbf{Y}^m_{lll}(\Omega\mathbf{r})\right) = 0, \tag{V22}$$

for any function h (σr). Eq. (V22) is independent of the origin of the coordinate system, i.e., it is valid also for $\mathbf{r}$-$\mathbf{r}_0$. Therefore, taking the gradient of Eq. (V1), we conclude that

$$\sum_{l'm'} \widetilde{W}_{lm;l'm'}(\mathbf{r}_0)\nabla^2\left(f_{l'}(\sigma r)Y_{l'm'}(\Omega\mathbf{r})\right) = 0 \tag{V23}$$

or

$$\sum_{l'm'} \widetilde{W}_{lm;l'm'}(\mathbf{r}_0) f_{l'}(\sigma r)Y_{l'm'}(\Omega\mathbf{r}) = 0\,. \tag{V24}$$

From the completeness of the spherical harmonics it follows that Eq. (V2c)is valid. Also, from Eq. (V21b) we obtain the identity

$$A_{lm;l'm'}(\mathbf{r}_0) + B_{lm;l'm'}(\mathbf{r}_0) = 0\,, \tag{v25}$$

and Eq. (V21a) becomes equal to

$$\widetilde{U}_{lm;l'm'}(\mathbf{r}_0) = \frac{2l'+1}{[l(l+1)l'(l'+1)]^{1/2}}(-1)^{m'}B_{lm;l'm'}(\mathbf{r}_0)\,, \tag{V26}$$

which is identical to Eq. (V2b).

Appendix VI

First, we shall compute the Fourier transform of $f_l(\sigma r)Y_{lm}(\Omega_r)$ inside the volume V_0 of radius R, and the Fourier transform of $g_l(\sigma r)Y_{lm}(\Omega_r)$ outside the volume V_0. For this purpose, we use the identity

$$e^{j\boldsymbol{\lambda}\cdot\mathbf{r}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_l(j\lambda r)Y^*_{lm}(\Omega_r)Y_{lm}(\Omega_\lambda) \tag{VI1}$$

where λ is the magnitude of $\boldsymbol{\lambda}$. Due to the orthonormality of the spherical harmonics, we obtain the following two relations:

$$\int_{V_0} f_l(\sigma r)Y_{lm}(\Omega_r)e^{j\boldsymbol{\lambda}\cdot\mathbf{r}}d^3x = 4\pi Y_{lm}(\Omega_\lambda)\int_0^R f_l(\sigma r)f_l(j\lambda r)r^2dr, \tag{VI2a}$$

$$\int_{V_\infty - V_0} g_l(\sigma r)Y_{lm}(\Omega_r)e^{j\boldsymbol{\lambda}\cdot\mathbf{r}}d^3x = 4\pi Y_{lm}(\Omega_\lambda)\int_R^\infty g_l(\sigma r)f_l(j\lambda r)r^2dr. \tag{VI2b}$$

The two integrals over r above are equal to

$$\int_0^R f_l(\sigma r)f_l(j\lambda r)r^2dr = \frac{R}{\lambda^2+\sigma^2}F_l(\lambda,\sigma), \tag{VI3a}$$

$$F_l(\lambda,\sigma) = \sigma R f_{l-1}(\sigma R)f_l(j\lambda R) - j\lambda R f_l(\sigma R)f_{l-1}(j\lambda R) \tag{VI3b}$$

and

$$\int_R^\infty g_l(\sigma r)f_l(j\lambda r)r^2dr = \frac{R}{\lambda^2+\sigma^2}G_l(\lambda,\sigma), \tag{VI4a}$$

where

$$G_l(\lambda,\sigma) = \sigma R g_{l-1}(\sigma R)f_l(j\lambda R) + j\lambda R g_l(\sigma R)f_{l-1}(j\lambda R) \tag{VI4b}$$

Then, the final result is as follows:

$$\int_{V_0} f_l(\sigma r)Y_{lm}(\Omega\mathbf{r})e^{j\boldsymbol{\lambda}\cdot\mathbf{r}}d^3x = \frac{4\pi R}{\lambda_z^2+\gamma^2}F_l(\lambda,\sigma)Y_{lm}(\Omega\lambda), \tag{VI5a}$$

$$\int_{V_\infty - V_0} g_l(\sigma r)Y_{lm}(\Omega\mathbf{r})e^{j\boldsymbol{\lambda}\cdot\mathbf{r}}d^3x = \frac{4\pi R}{\lambda_z^2+\gamma^2}G_l(\lambda,\sigma)Y_{lm}(\Omega_\lambda), \tag{VI5b}$$

where

$$\gamma = \left[\lambda_\rho^2 + \sigma^2\right]^{1/2}, \tag{VI6a}$$

$$\lambda_\rho = \left[\lambda_x^2 + \lambda_y^2\right]^{1/2}. \tag{VI6b}$$

Next, we shall compute the Fourier transforms of the vector functions in Eqs. (55a), (55b), which we define as follows:

$$\hat{\mathbf{E}}_{2,lm}^{(M,in)}(\lambda) = \int_{V_0} \mathbf{E}_{2,lm}^{(M,in)}(\mathbf{r}) e^{j\lambda\cdot\mathbf{r}} d^3x, \tag{VI7a}$$

$$\hat{\mathbf{E}}_{2,lm}^{(\alpha,out)}(\lambda) = \int_{V_\infty - V_0} \mathbf{E}_{2,lm}^{(\alpha,out)}(\mathbf{r}) e^{j\lambda\cdot\mathbf{r}} d^3x, \tag{VI7b}$$

where α=M or E. The vector function $\mathbf{E}_{2,lm}^{(M,in)}(\mathbf{r})$ is given by Eq. (10a), and $\mathbf{E}_{2,lm}^{(\alpha,out)}(\mathbf{r})$ is given by Eqs. (40a), (40b). Then, with the help of Eqs. (I2a), (I10a) and the Fourier transforms just computed, it is rather easy to show that

$$\hat{\mathbf{E}}_{2,lm}^{(M,in)}(\lambda) = \frac{4\pi R}{\lambda_z^2 + \gamma_2^2} F_l(\lambda, \sigma_2) \mathbf{Y}_{lll}^m(\Omega_\lambda), \tag{VI8a}$$

$$\hat{\mathbf{E}}_{2,lm}^{(M,out)}(\lambda) = \frac{4\pi R}{\lambda_z^2 + \gamma_2^2} G_l(\lambda, \sigma_2) \mathbf{Y}_{lll}^m(\Omega_\lambda), \tag{VI8b}$$

$$\hat{\mathbf{E}}_{2,lm}^{(E,out)}(\lambda) = -\frac{4\pi R}{\lambda_z^2 + \gamma_2^2}\left[\left(\frac{l}{2l+1}\right)^{1/2} G_{l+1}(\lambda, \sigma_2) \mathbf{Y}_{l,l+1,l}^m(\Omega_\lambda) + \left(\frac{l+1}{2l+1}\right)^{1/2} G_{l-1}(\lambda, \sigma_2) \mathbf{Y}_{l,l-1,l}^m(\Omega_\lambda)\right], \tag{VI8c}$$

where

$$\gamma_2 = \left[\lambda_\rho^2 + \sigma_2^2\right]^{1/2}. \tag{VI9}$$

Equ. (IV8c) can also be written as follows:

$$\hat{\mathbf{E}}_{2,lm}^{(E,out)}(\lambda) = \frac{1}{j\sigma_2}(-j\lambda) \times \mathbf{E}_{2,lm}^{(M,out)}(\lambda) + \frac{4\pi R}{\sigma_2} g_l(\sigma_2 R) \nabla_\lambda \times \left(f_l(j\lambda R) \mathbf{Y}_{lll}^m(\Omega_\lambda)\right). \tag{VI10}$$

Appendix VII

We shall prove Eq. (99), where we set $\sigma_2=\sigma$, here. From the integral form of $\widetilde{G}_{lm;l'm'}(\mathbf{a}_{pq})$, i.e., Eq. (IV10), and the Fourier transforms of $g_l(\sigma r)Y_{lm}(\Omega_\lambda), f_l(\sigma r)Y_{lm}(\Omega_\lambda)$, i.e., Eqs. (VI5a), (VI5b), we obtain the relation

$$\widetilde{G}_{lm;l'm'}(\mathbf{a}_{pq})=\frac{2R^2}{\pi\zeta_{l'}}\int\frac{F_{l'}^*(\lambda,\sigma)}{\lambda_z^2+\gamma^{*2}}\frac{G_l(\lambda,\sigma)}{\lambda_z^2+\gamma^2}Y_{l'm'}^*(\Omega_\lambda)Y_{lm}(\Omega_\lambda)e^{j\lambda\cdot\mathbf{a}_{pq}}d^3\lambda\,, \qquad \text{(VII1)}$$

the integration extending over the whole volume in the spectral domain. Substitution of this relation into Eq. (92) and making use of the transition relation given by Eq. (68) leads to the validity of Eq. (99). Notice that the prime in Eq. (92) can be removed when the integral form of $\widetilde{G}_{lm;l'm'}(\mathbf{a}_{pq})$ is used (cf. statement before Eq. (94a)).

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